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FILE 'REGISTRY' ENTERED AT 18:03:54 ON 28 JAN 2008
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STRUCTURE FILE UPDATES:   27 JAN 2008  HIGHEST RN 1000849-38-6
DICTIONARY FILE UPDATES:  27 JAN 2008  HIGHEST RN 1000849-38-6

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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  conducting SmartSELECT searches.

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predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> d que sta l9
L5              STR

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VAR G1=AK/CB
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E6 C  E1 N  AT   1
ECOUNT  IS E4 C  E2 N  AT   2

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
L7         3902 SEA FILE=REGISTRY ABB=ON  PLU=ON  NCNC3/ES AND NC6/ES
L9          301 SEA FILE=REGISTRY SUB=L7 SSS FUL L5

100.0% PROCESSED    3902 ITERATIONS                          301 ANSWERS
SEARCH TIME: 00.00.01



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L25             STR

Hy^Hy--N
 1   2   3


NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED
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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
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SEARCH TIME: 00.00.01
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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 28 Jan 2008  VOL 148 ISS 5
FILE LAST UPDATED: 27 Jan 2008  (20080127/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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L12 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:515487 HCAPLUS
DN 141:71555
TI Preparation of nitrogen-containing heterocyclic compounds as CXCR4 regulators
IN Habashita, Hiromu; Kokubo, Masaya; Shibayama, Shiro; Tada, Hideaki; Tanihiro, Tatsuya
PA Ono Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 641 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2004052862	A1	20040624	2003WO-JP15718	20031209
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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PRAI 2002JP-0357446	A	20021210		
2003JP-0162706	A	20030606		
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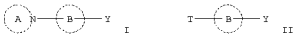
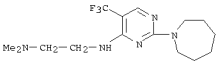
OS MARPAT 141:71555
GI



AB Compds. such as pyrimidine and quinazoline derivs. represented by the following general formulas (I) and (II), salts thereof, N-oxides thereof, solvates thereof or prodrugs of the same (wherein the ring A represents an optionally substituted nitrogen-containing heterocycle; the ring B represents an optionally substituted homocycle or an optionally substituted heterocycle; Y represents an optionally substituted hydrocarbyl group, an optionally substituted heterocyclic group, an optionally protected amino group, an optionally protected hydroxyl group or an optionally protected mercapto group; and T represents the ring A or an optionally substituted amino group) are prepared These compds. are CXCR4 regulators, in particular CXCR4 antagonists, and useful as preventives and/or remedies for various inflammatory diseases, immune diseases, various allergic diseases, infectious diseases, acquired immunodeficiency syndrome, infection with human immunodeficiency virus, psychiatric disorder, neurol. disease, cerebral diseases, cardiovascular diseases, metabolic diseases, or cancer, and agents for regeneration therapy, in particular transplant therapy. An assay system using SDF-1 which is an endogenous ligand of CXCR4 receptor, instead of HIV, was used in an assay for screening compds. which inhibit the binding of HIV to CXCR4 or CCR4 receptors on CD4-pos. cells. All the compds. prepared showed IC50 of 10 μM for inhibiting the binding of [125I]human SDF-1 to CEM cells, more specifically 0.1 μM for 2-(1-benzylpyrrolidin-3-ylamino)-4-(perhydroazepin-1-yl)pyrimidine. An ampule and tablet formulation containing 2-{[2-(dimethylamino)ethyl]amino}-4-(perhydroazepin-1-yl)pyrimidine were described.
IT 710998-66-6P 710998-67-7P 710998-68-8P
710999-88-5P 710999-91-0P 710999-92-1P
711000-15-6P 711000-16-7P 711000-17-8P

L12 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
711000-18-9P 711001-26-2P 711001-73-9P
711001-74-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)
IT 710998-66-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogen-containing heterocyclic compds. as CXCR4 antagonists for preparation and/treatment of diseases)
RN 710998-66-6 HCAPLUS
CN 1,2-Ethanediamine, N'-[2-(hexahydro-1H-azepin-1-yl)-5-(trifluoromethyl)-4-pyrimidinyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



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=> d bib abs hitstr l35 tot
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L35 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:515487 HCAPLUS
DN 141:71555
TI Preparation of nitrogen-containing heterocyclic compounds as CXCR4 regulators
IN Habashita, Hiromu; Kokubo, Masaya; Shibayama, Shiro; Tada, Hideaki; Tanihiro, Tatsuya
PA Ono Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 641 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2004052862	A1	20040624	2003WO-JP15718	20031209
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU2003288994	A1	20040630	2003AU-0288994	20031209
EP---1571146	A1	20050907	2003EP-0778753	20031209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US2007167459	A1	20070719	2005US-0538758	20050610
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2003JP-0162706	A	20030606		
2003WO-JP15718	W	20031209		

OS MARPAT 141:71555
GI

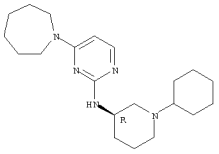
I II

AB Compds. such as pyrimidine and quinazoline derivs. represented by the following general formulas (I) and (II), salts thereof, N-oxides thereof, solvates thereof or prodrugs of the same (wherein the ring A represents an optionally substituted nitrogen-containing heterocycle; the ring B represents an optionally substituted homocycle or an optionally substituted heterocycle; Y represents an optionally substituted hydrocarbyl group, an optionally substituted heterocyclic group, an optionally protected amino group, an optionally protected hydroxyl group or an optionally protected mercapto group; and T represents the ring A or an optionally substituted amino group) are prepared These compds. are CXCR4 regulators, in particular CXCR4 antagonists, and useful as preventives and/or remedies for various inflammatory diseases, immune diseases, various allergic diseases, infectious diseases, acquired immunodeficiency syndrome, infection with human immunodeficiency virus, psychiatric disorder, neurol. disease, cerebral diseases, cardiovascular diseases, metabolic diseases, or cancer, and agents for regeneration therapy, in particular transplant therapy. An assay system using SDF-1 which is an endogenous ligand of CXCR4 receptor, instead of HIV, was used in an assay for screening compds. which inhibit the binding of HIV to CXCR4 or CCR4 receptors on CD4-pos. cells. All the compds. prepared showed IC50 of 10 μM for inhibiting the binding of [125I]human SDF-1 to CEM cells, more specifically 0.1 μM for 2-(1-benzylpyrrolidin-3-ylamino)-4-(perhydroazepin-1-yl)pyrimidine. An ampule and tablet formulation containing 2-{[2-(dimethylamino)ethyl]amino}-4-(perhydroazepin-1-yl)pyrimidine were described.

IT 710986-02-0P 711006-64-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

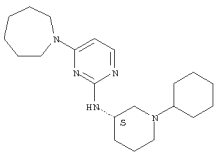
L35 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
(Uses)
(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)
RN 710986-02-0 HCAPLUS
CN 2-Pyrimidinamine, N-[(3R)-1-cyclohexyl-3-piperidinyl]-4-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

Absolute stereochemistry.



RN 711006-64-3 HCAPLUS
CN 2-Pyrimidinamine, N-[(3S)-1-cyclohexyl-3-piperidinyl]-4-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

Absolute stereochemistry.



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L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:610405 HCAPLUS
DN 137:169534
TI Preparation of imidazolyl pyrimidinamines as NOS inhibitors
IN Arnaiz, Damian O.; Baldwin, John J.; Davey, David D.; Devlin, James J.; Dolle, Roland Ellwood, III; Erickson, Shawn David; McMillan, Kirk; Morrissey, Michael M.; Ohlmeyer, Michael H. J.; Pan, Gonghua; Paradkar, Vidyadhar Madhav; Parkinson, John; Phillips, Gary B.; Ye, Bin; Zhao, Zuchun
PA Berlex Laboratories, Inc., USA; Pharmacopeia, Inc.
SO U.S., 132 pp., Cont.-in-part of U.S. Ser. No. 25,124, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US---6432947	B1	20020813	1999US-0383813	19990826 <--
CN---1100777	B	20030205	1998CN-0804281	19980219 <--
AT----345339	T	20061215	1998AT-0906555	19980219 <--
EP---1754703	A2	20070221	2006EP-0023449	19980219 <--
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L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

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1998US-0025124 B2 19980217 <--
1998EP-0906555 A3 19980219 <--
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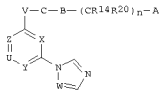
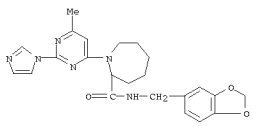


I

AB The title compds. [I; U = N, CR5 (R5 = H, halo, alkyl, optionally substituted aralkyl or aryl, etc.); V = NR4, S, O, CHR4 (R4 = H, alkyl, aryl, aralkyl, cycloalkyl); W = N, CH; X, Y, Z = N, CR19 (R19 = H, alkyl, cyclopropyl, halo, haloalkyl); A = R1, OR1, CONR1R2, PO(NR1R2)2, NR1COR2, etc. (R1, R2 = H, optionally substituted alkyl or cycloalkyl, etc. or NR1R2 = N-heterocyclyl); B = CR17(CHR15)mQR3 (m = 1-4, R3 = H, alkyl, cycloalkyl, optionally substituted aryl, etc.; R15, R17 = H, alkyl; Q = CO, O, C:NR1, etc.); C = (CHR12)q(CHR13)r (q, r = 0-1; R12, R13 = H, alkyl); or B = C = null; R14, R20 = H, alkyl; n = 1-3], useful as inhibitors of nitric oxide synthase, were prepared Thus, N-[(1,3-benzodioxol-5-yl)methyl]-1-[3-(1H-imidazol-1-yl)phenyl]piperidine-2-acetamide was prepared by reaction of 1-(3-aminophenyl)imidazole, Et 7-chloro-3-oxoheptanoate, and piperonylamine. All exemplified compds. I showed iNOS inhibitory activity at concns. less than 25 μM.

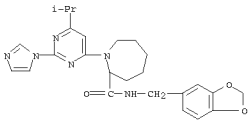
IT 212650-00-5P 212650-01-6P 212650-03-8P
212650-05-0P 212650-06-1P 212650-09-4P
212650-11-8P 212650-12-9P 212650-13-0P
212650-15-2P 212650-16-3P 212650-18-5P
212650-19-6P 212650-20-9P 212650-21-0P
212650-22-1P 212650-24-3P 212650-26-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of imidazolyl pyrimidinamines as NOS inhibitors)

RN 212650-00-5 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-(1,3-benzodioxol-5-ylmethyl)hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 212650-01-6 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-(1,3-benzodioxol-5-ylmethyl)hexahydro-1-[2-(1H-imidazol-1-yl)-6-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)



RN 212650-03-8 HCAPLUS
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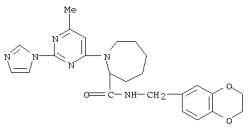

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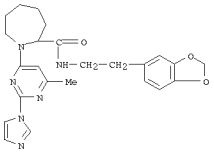
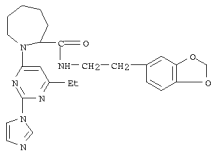
CN 1H-Azepine-2-carboxamide, N-[2-(1,3-benzodioxol-5-yl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)

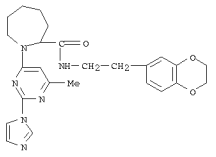


RN 212650-06-1 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-[2-(1,3-benzodioxol-5-yl)ethyl]-1-[6-ethyl-2-(1H-imidazol-1-yl]-4-pyrimidinyl]hexahydro- (CA INDEX NAME)

L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-09-4 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



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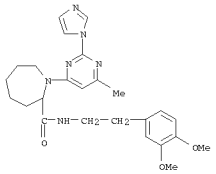

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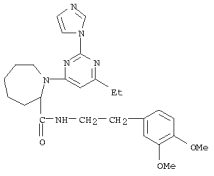
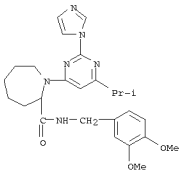
CN 1H-Azepine-2-carboxamide, N-[2-(3,4-dimethoxyphenyl)ethyl]-1-[6-ethyl-2-(1H-imidazol-1-yl]-4-pyrimidinyl]hexahydro- (CA INDEX NAME)

L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-13-0 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-[(3,4-dimethoxyphenyl)methyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)



RN 212650-15-2 HCAPLUS
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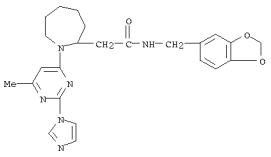

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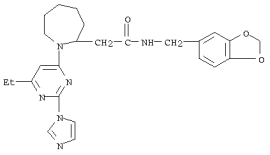
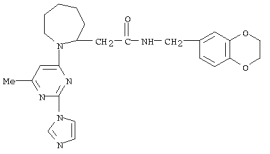
L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-18-5 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



RN 212650-19-6 HCAPLUS
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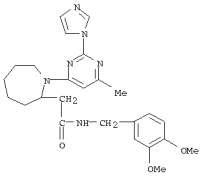
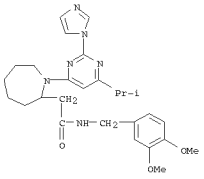
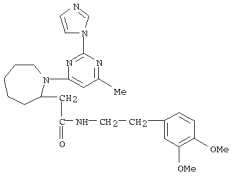


RN 212650-20-9 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[(3,4-dimethoxyphenyl)methyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)

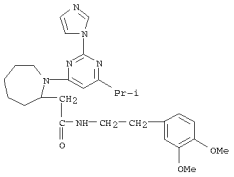
L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-21-0 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[2-(3,4-dimethoxyphenyl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)

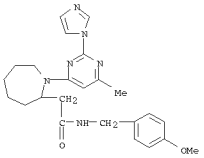


RN 212650-22-1 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[2-(3,4-dimethoxyphenyl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)

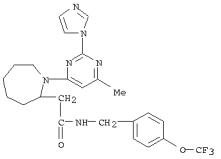


RN 212650-24-3 HCAPLUS
CN 1H-Azepine-2-acetamide, hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]-N-[(4-methoxyphenyl)methyl]- (CA INDEX NAME)

L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-26-5 HCAPLUS
CN 1H-Azepine-2-acetamide, hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]-N-[[4-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 1998:604917 HCAPLUS
DN 129:231019
TI Preparation of N-heterocyclic derivatives as NOS inhibitors
IN Arnaiz, Damian O.; Baldwin, John J.; Davey, David D.; Devlin, James J.; Dolle, Roland Ellwood, III; Erickson, Shawn David; McMillan, Kirk; Morrissey, Michael M.; Ohlmeyer, Michael H. J.; Pan, Gonghua; Paradkar, Vidyadhar Madhav; Parkinson, John; Phillips, Gary B.; Ye, Bin; Zhao, Zuchun; et al.
PA Berlex Laboratories, Inc., USA; Pharmacopeia, Inc.; et al.
SO PCT Int. Appl., 358 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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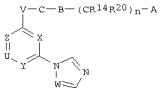

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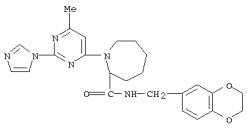
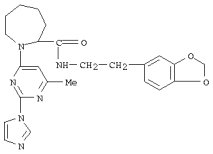
L19 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-05-0 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-[2-(1,3-benzodioxol-5-yl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



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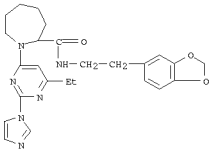

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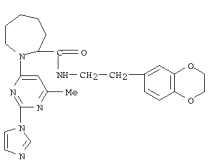
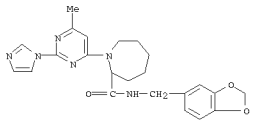
CN 1H-Azepine-2-carboxamide, N-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)

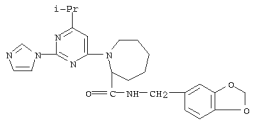


L19 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

AB N-Heterocyclic derivs. I [U = N, CR5 (R5 = H, halo, alkyl, optionally substituted aralkyl or aryl, etc.); V = NR4, S, O, CHR4 (R4 = H, alkyl, aryl, aralkyl, cycloalkyl); W = N, CH; X, Y, Z = N, CR19 (R19 = H, alkyl, cyclopropyl, halo, haloalkyl); A = R1, OR1, CONR1R2, PO(NR1R2)2, NR1COR2, etc. (R1, R2 = H, optionally substituted alkyl or cycloalkyl, etc. or R1R2N = N-heterocyclyl); B = CR17(CHR15)mQR3 (m = 1-4, R3 = H, alkyl, cycloalkyl, optionally substituted aryl, etc.; R15, R17 = H, alkyl; Q = CO, O, C:NR1, etc.); N-heterocyclyl; C = (CHR12)q(CHR13)r (q, r = 0 or 1; R12, R13 = H, alkyl); or B = C = null; R14, R20 = H, alkyl; n = 1-3] were prepared as inhibitors of nitric oxide synthase. Thus, N-[(1,3-benzodioxol-5-yl)methyl]-1-[3-(1H-imidazol-1-yl)phenyl]piperidine-2-acetamide was prepared by reaction of 1-(3-aminophenyl)imidazole, 7-chloro-3-oxoheptanoic acid Et ester, and piperonylamine.
IT 212650-00-5P 212650-01-6P 212650-03-8P
212650-05-0P 212650-06-1P 212650-09-4P
212650-11-8P 212650-12-9P 212650-13-0P
212650-15-2P 212650-16-3P 212650-18-5P
212650-19-6P 212650-20-9P 212650-21-0P
212650-22-1P 212650-24-3P 212650-26-5P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-heterocyclic derivs. as NOS inhibitors)
RN 212650-00-5 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-(1,3-benzodioxol-5-ylmethyl)hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



RN 212650-01-6 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-(1,3-benzodioxol-5-ylmethyl)hexahydro-1-[2-(1H-imidazol-1-yl)-6-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)



RN 212650-03-8 HCAPLUS
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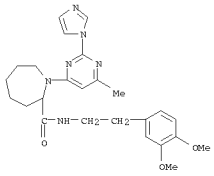
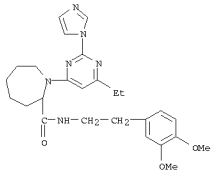
L19 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

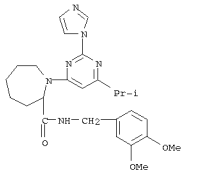
RN 212650-11-8 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-[2-(3,4-dimethoxyphenyl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



RN 212650-12-9 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-[2-(3,4-dimethoxyphenyl)ethyl]-1-[6-ethyl-2-(1H-imidazol-1-yl)-4-pyrimidinyl]hexahydro- (CA INDEX NAME)

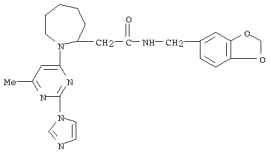


RN 212650-13-0 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-[(3,4-dimethoxyphenyl)methyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)

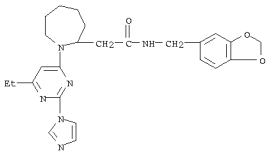


RN 212650-15-2 HCAPLUS
CN 1H-Azepine-2-acetamide, N-(1,3-benzodioxol-5-ylmethyl)hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)

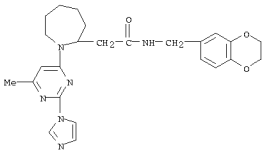
L19 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-16-3 HCAPLUS
CN 1H-Azepine-2-acetamide, N-(1,3-benzodioxol-5-ylmethyl)-1-[6-ethyl-2-(1H-imidazol-1-yl)-4-pyrimidinyl]hexahydro- (CA INDEX NAME)

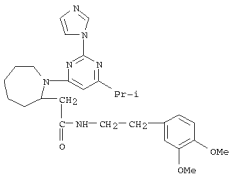


RN 212650-18-5 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



RN 212650-19-6 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[(3,4-dimethoxyphenyl)methyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)

L19 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-24-3 HCAPLUS
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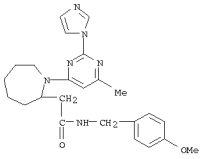
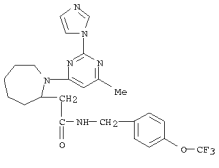
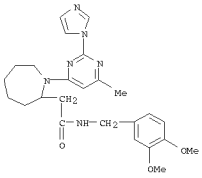


RN 212650-26-5 HCAPLUS
CN 1H-Azepine-2-acetamide, hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]-N-[[4-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)

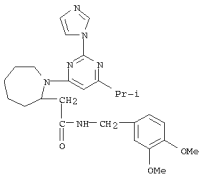


RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

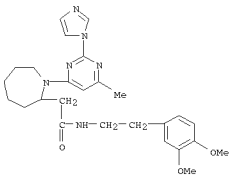
L19 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-20-9 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[(3,4-dimethoxyphenyl)methyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)



RN 212650-21-0 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[2-(3,4-dimethoxyphenyl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



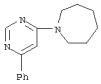
RN 212650-22-1 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[2-(3,4-dimethoxyphenyl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)

L19 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1976:478153 HCAPLUS
DN 85:78153
ORER 85:12561a,12564a
TI 4-Amino-6-arylpyrimidines and salts useful for relaxation of smooth muscle in a mammal
IN De Angelis, Gerald G.; Hess, Hans J. E.
PA Pfizer Inc., USA
SO U.S., 25 pp. Division of U.S. 3,895,112.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US---3950525	A	19760413	1975US-0567356	19750411 <--
	US---3859288	A	19750107	1971US-0182220	19710920 <--
	US---3895112	A	19750715	1973US-0371483	19730619 <--
PRAI	1971US-0182220	A3	19710920	<--	
	1973US-0371483	A3	19730619	<--	
	1975US-0078216	A2	19751005	<--	
	1970US-0078216	A2	19701005	<--	

GI

AB Pyrimidinamines I (R = Ph, substituted phenyl, furyl, thienyl, naphthyl; R1 and R2 = H, alkyl, hydroxyalkyl, aminoalkyl; NR1R2 = heterocyclic; R3 = H, Me, Et, Pr, CHMe2) (100 compds.) were prepared and have platelet aggregation-inhibiting and bronchodilator properties. Thus, I (R = Ph, R1 = R2 = Et, R3 = H) were obtained by Grignard reaction of PhBr with NCCH2CO2Et, condensation of H2NCPh:CHCO2Et with HCONH2, chlorination of 4-hydroxy-6-phenylpyrimidine, and amination of the 4-chloro compound
IT 36822-82-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36822-82-9 HCAPLUS
CN 1H-Azepine, hexahydro-1-(6-phenyl-4-pyrimidinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

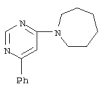


● HCl

L19 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1976:59528 HCAPLUS
DN 84:59528
OREF 84:9803a,9806a
TI Arylpyrimidines, inhibitors of platelet aggregation and bronchodilators
IN De Angelis, Gerald G.; Hess, Hans J. E.
PA Pfizer Inc., USA
SO U.S., 27 pp. Division of U.S. 3,859,288.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 4

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US---3908012	A	19750923	1973US-0371420	19730619 <--
US---3707560	A	19721226	1970US-0078216	19701005 <--
US---3859288	A	19750107	1971US-0182220	19710920 <--
DK----130971	B	19750512	1973DK-0001429	19730316 <--
US---3890321	A	19750617	1973US-0371563	19730619 <--
CA----978531	A2	19751125	1973CA-0176049	19730710 <--
CA----978532	A2	19751125	1974CA-0191086	19740128 <--
FI-----55834	C	19791010	1977FI-0003287	19771102 <--
FI-----55834	B	19790629		
PRAI 1970US-0078216	A2	19701005	<--	
1971US-0182220	A3	19710920	<--	
1971FI-0002734	A	19710930	<--	
1971DK-0004801	A	19711001	<--	
1971CA-0124312	A3	19711004	<--	

GI For diagram(s), see printed CA Issue.
AB About 100 pyrimidines I (R = Ph, p-ClC6H4, 2-furyl, 2-thienyl, 3-H2NC6H4, etc., R1 = H, Me, Et, Pr; R2 = Et2N, MeNH, Bu2N, 1-pyrrolidinyl, piperidino, etc.) were prepared by substitution of I (R = Cl) or treating chlorobenzothienopyrimidines with amines followed by cleaving. Thus, NCCH2CO2Et was treated with PhMgBr and the H2NCPh:CHCO2Et cyclized with HCONH2 to give I (R = Ph, R1 = H, R2 = OH), which was chlorinated with POCl3 and treated with Et2NH to give I (R = Ph, R1 = H, R2 = Et2N). At 10-4 μ I (R = Ph, R1 = H, R2 = Et2N) inhibited in vitro platelet aggregations by 99%. At 60 mg/kg I (R = 3-O2NC6H4, R1 = H, R2 = Et2N) gave 20% protection against histamine induced bronchoconstriction in guinea pigs.
IT 36822-82-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and platelet aggregation inhibition of)
RN 36822-82-9 HCAPLUS
CN 1H-Azepine, hexahydro-1-(6-phenyl-4-pyrimidinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

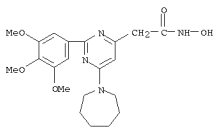


● HCl

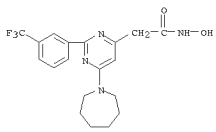
L19 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1975:171040 HCAPLUS
DN 82:171040
OREF 82:27345a,27348a
TI 6-Pyrimidinylacethydroxamic acids
IN Fauran, Claude; Eberle, Jeannine; Bourgery, Guy; Raynaud, Guy; Gouret, Claude
PA Delalande S. A., Fr.
SO Fr. Demande, 13 pp. Addn. to Fr. 2,158,081 (See Ger. 2,252,822, CA 79;32093c).
CODEN: FRXXBL
DT Patent
LA French
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI FR---2225154	A2	19741108	1973FR-0013667	19730416 <--
FR---2225154	B2	19760702		
PRAI 1973FR-0013667	A	19730416	<--	

GI For diagram(s), see printed CA Issue.
AB Analgesic and antiinflammatory (no data) pyrimidinylacethydroxamic acids I (NRR1 = NMe2, NEt2, pyrrolidino, piperidino, hexamethylenimino, morpholino; R2 = NHOH; R3 = 3-FC6H4, 3-ClC6H4, 3,4,5-(MeO)3C6H2, 3-CF3C6H4, 3,4-methylenedioxyphenyl) were prepared by treating I (R2 = OEt) with NH2OH.
IT 42055-69-6P 42055-79-8P 55675-39-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42055-69-6 HCAPLUS
CN 4-Pyrimidineacetamide, 6-(hexahydro-1H-azepin-1-yl)-N-hydroxy-2-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)

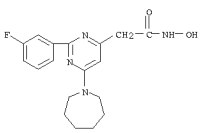


RN 42055-79-8 HCAPLUS
CN 4-Pyrimidineacetamide, 6-(hexahydro-1H-azepin-1-yl)-N-hydroxy-2-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

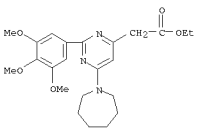


RN 55675-39-3 HCAPLUS
CN 4-Pyrimidineacetamide, 2-(3-fluorophenyl)-6-(hexahydro-1H-azepin-1-yl)-N-hydroxy- (CA INDEX NAME)

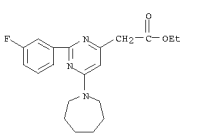
L19 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



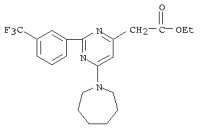
IT 42055-86-7 55675-45-1 55675-47-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydroxylamine)
RN 42055-86-7 HCAPLUS
CN 4-Pyrimidineacetic acid, 6-(hexahydro-1H-azepin-1-yl)-2-(3,4,5-trimethoxyphenyl)-, ethyl ester (CA INDEX NAME)



RN 55675-45-1 HCAPLUS
CN 4-Pyrimidineacetic acid, 2-(3-fluorophenyl)-6-(hexahydro-1H-azepin-1-yl)-, ethyl ester (CA INDEX NAME)



RN 55675-47-3 HCAPLUS
CN 4-Pyrimidineacetic acid, 6-(hexahydro-1H-azepin-1-yl)-2-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

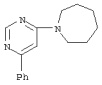


L19 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1972:448506 HCAPLUS
DN 77:48506
OREF 77:8051a,8054a
TI 6-Arylpyrimidines for inhibiting thrombocyte aggregation and as bronchodilators
IN De Angelis, Gerald G.; Hess, Hans J. E.
PA Pfizer Inc.
SO Ger. Offen., 87 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 4

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE---2149249	A	19720413	1971DE-2149249	19711002 <--
DE---2149249	B2	19741107		
DE---2149249	C3	19750703		
US---3707560	A	19721226	1970US-0078216	19701005 <--
FI-----55502	C	19790810	1971FI-0002734	19710930 <--
FI-----55502	B	19790430		
DK----131858	B	19750915	1971DK-0004801	19711001 <--
ZA---7106615	A	19720628	1971ZA-0006615	19711004 <--
ES----395676	A1	19741016	1971ES-0395676	19711004 <--
GB---1373535	A	19741113	1971GB-0046158	19711004 <--
GB---1373536	A	19741113	1973GB-0038316	19711004 <--
CA----988519	A1	19760504	1971CA-0124312	19711004 <--
SE----385885	C	19761104	1971SE-0012534	19711004 <--
SE----385885	B	19760726		
SE----390304	B	19761213	1974SE-0010488	19711004 <--
BE----773484	A1	19720405	1971BE-0003448	19711005 <--
NL---7113670	A	19720407	1971NL-0013670	19711005 <--
NL----168511	B	19811116		
NL----168511	C	19820416		
FR---2110227	A5	19720602	1971FR-0035815	19711005 <--
FR---2110227	B1	19750207		
CH----542218	A	19731115	1973CH-0007729	19711005 <--
AT----314540	B	19740410	1971AT-0008580	19711005 <--
AT----315856	B	19740610	1973AT-0000148	19711005 <--
AT----316563	B	19740725	1973AT-0000149	19711005 <--
AT----317229	B	19740826	1973AT-0006054	19711005 <--
CH----554346	A	19740930	1972CH-0015321	19711005 <--
CH----554876	A	19741015	1971CH-0014529	19711005 <--
CH----554875	A	19741015	1972CH-0015214	19711005 <--
JP--56048511	B	19811116	1971JP-0078237	19711005 <--
AU----7134259	A	19730412	1971AU-0034259	19711006 <--
DK----130971	B	19750512	1973DK-0001429	19730316 <--
CA----978531	A2	19751125	1973CA-0176049	19730710 <--
ES----420211	A1	19760316	1973ES-0420211	19731102 <--
ES----420209	A1	19760601	1973ES-0420209	19731102 <--
ES----420210	A1	19760601	1973ES-0420210	19731102 <--
CA----978532	A2	19751125	1974CA-0191086	19740128 <--
SE----7410488	A	19740816	1974SE-0010488	19740816 <--
FI-----55834	C	19791010	1977FI-0003287	19771102 <--
FI-----55834	B	19790629		
JP--56036468	A	19810409	1980JP-0110163	19800811 <--
JP--57008107	B	19820215		
PRAI 1970US-0078216	A	19701005	<--	
1971FI-0002734	A	19710930	<--	
1971DK-0004801	A	19711001	<--	
1971CA-0124312	A3	19711004	<--	

GI For diagram(s), see printed CA Issue.
AB 4-Amino-6-arylpyrimidines (I), useful for inhibition of thrombocyte aggregation and as bronchodilators, were prepared by reaction of RMgX with R1CH(CN)CO2Et to give ArC(NH2):CR1CO2Et, which was condensed with HCONH2 to give the 4-hydroxy analog of I, treated with POCl3, and R2R3NH. Other methods included reaction of substituted 6-chlorobenzonitrile with NaSCH2CO2Me to give 2-amino-3-methoxydihydrobenzo[b]thiophene which was condensed with HCONH2 to give a 4-hydroxy-[1]benzothieno[3,2-d]pyrimidine, treatment with POCl3, R2R3NH, then H over Raney Ni, or by condensation of RCOCHR1CO2Et with (NH2)2CS to give a 6-aryl-2-mercapto-4-hydroxypyrimidine which was hydrogenated over Raney Ni, treated with POCl3, then R2R3NH. About 75 I [R = Ph, substituted phenyl, 2-furyl, 2-thienyl; R1 = H, Et, Pr; R2 = H, C1-4 alkyl, allyl; R3 = H, C1-4 alkyl, CF3CH2, allyl, Me2N(CH2)2, 3-picolyl; or R2R3 = (CH2)4-6, (CH2)2O(CH2)2, or

L19 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
(CH2)2NMe(CH2)2] were prepd.
IT 36822-82-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36822-82-9 HCAPLUS
CN 1H-Azepine, hexahydro-1-(6-phenyl-4-pyrimidinyl)-, monohydrochloride (9CI)
(CA INDEX NAME)



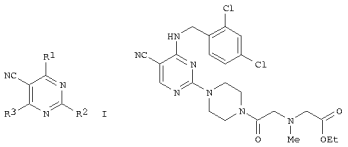
● HCl

=> d bib abs hitind hitstr l40 tot

L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:796691 HCAPLUS
DN 139:307788
TI Preparation of 5-cyanopyrimidine derivatives as anti-inflammatory agents
IN Machii, Daisuke; Yamaura, Yosuke; Arai, Hitoshi; Yanagawa, Koji; Ohshima, Etsuo; Kawanabe, Ari; Iwase, Miho; Kobayashi, Katsuya; Sato, Takashi; Miki, Ichiro
PA Kyowa Hakko Kogyo Co., Ltd., Japan
SO PCT Int. Appl., 169 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2003082855	A1	20031009	2003WO-JP04009	20030328
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU2003220968	A1	20031013	2003AU-0220968	20030328
PRAI 2002JP-0090640	A	20020328		
2003WO-JP04009	W	20030328		

OS MARPAT 139:307788
GI



AB The title pyrimidine compds. I [wherein R1 and R3 = independently H, OH, halo, (un)substituted alkyl, alkoxy, alkylthio, aryl, aralkyl, or amino; R2 = (un)substituted amino) or ammonium salts or pharmaceutically acceptable salts thereof are prepared as anti-inflammatory agents. For example, the compound II was prepared in a multi-step synthesis. II showed 97% inhibitory activity against thymus and activation-regulated chemokine (TARC) Hut78 cells at 1 μM. Formulations containing I as an active ingredient were also described.
IC ICM C07D-401/12
ICS C07D-239/42; C07D-401/04; C07D-405/12; C07D-413/04; C07D-401/14; C07D-403/12; C07D-403/04; A61K-031/506; A61K-031/5377; A61K-031/541; A61K-031/55; A61P-029/00; A61P-037/08; A61P-043/00
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
IT Chemokines
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(thymus and activation-regulated, macrophage-derived; preparation of cyanopyrimidine derivs. as anti-inflammatory agents)
IT 611199-85-0P 611199-86-1P 611199-87-2P 611199-88-3P 611199-89-4P
611199-90-7P 611199-91-8P 611199-92-9P 611199-93-0P 611199-94-1P

L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
611199-95-2P 611199-96-3P 611199-97-4P 611199-98-5P 611199-99-6P
611200-00-1P 611200-01-2P 611200-02-3P 611200-03-4P 611200-04-5P
611200-05-6P 611200-06-7P 611200-08-9P 611200-09-0P 611200-10-3P
611200-11-4P 611200-12-5P 611200-13-6P 611200-14-7P 611200-15-8P
611200-16-9P 611200-17-0P 611200-18-1P 611200-19-2P 611200-20-5P
611200-21-6P 611200-22-7P 611200-23-8P 611200-24-9P 611200-25-0P
611200-26-1P 611200-27-2P 611200-28-3P 611200-29-4P 611200-30-7P
611200-31-8P 611200-32-9P 611200-33-0P 611200-34-1P 611200-35-2P
611200-36-3P 611200-37-4P 611200-38-5P 611200-39-6P
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611200-58-9P 611200-59-0P 611200-60-3P 611200-61-4P 611200-62-5P
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611200-88-5P 611200-89-6P 611200-90-9P 611200-91-0P 611200-92-1P
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L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
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(drug candidate; preparation of cyanopyrimidine derivs. as anti-inflammatory agents)
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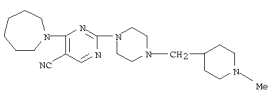

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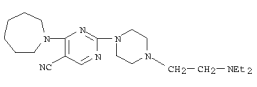

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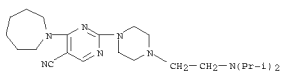
L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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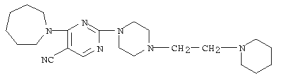

RN 611200-44-3 HCAPLUS
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RN 611200-45-4 HCAPLUS
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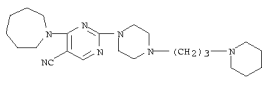

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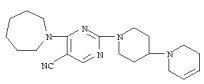

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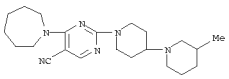
L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 611201-16-2 HCAPLUS
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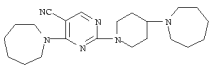

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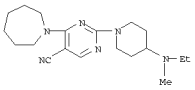

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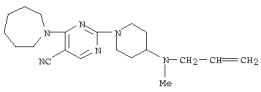
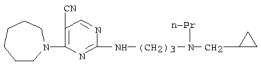
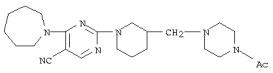


RN 611202-14-3 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 2-[[3-[(cyclopropylmethyl)propylamino]propyl]amino]-4-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)



RN 611202-85-8 HCAPLUS
CN Piperazine, 1-acetyl-4-[[1-[5-cyano-4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]-3-piperidinyl]methyl]- (9CI) (CA INDEX NAME)

L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 611204-30-9 HCAPLUS
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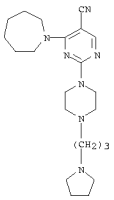

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L2              TRA L1 1- RN :     1829 TERMS

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L4           1375 L3 AND NC6/ES AND  46.195.39/RID
L5              STR
L6              0 L5
L7           3902 NCNC3/ES AND NC6/ES
L8              7 L5 SAM SUB=L7
L9            301 L5 FULL SUB=L7
                SAV TEM J758C1/A L9
L10            13 L9 AND L3

     FILE 'HCAPLUS' ENTERED AT 17:11:20 ON 28 JAN 2008

     FILE 'REGISTRY' ENTERED AT 17:11:22 ON 28 JAN 2008
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L14            61 L13 AND (PD<=20031209 OR AD<=20031209 OR PRD<=20031209)
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L20             0 L17

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                E CHEMOKINE RECEPTORS/CT
                E E3+ALL
L21         13030 E19+OLD
                E E22+ALL
L22         27324 E10+OLD,NT
L23             2 L21-22 AND L13
                SEL HIT RN 2
                SEL AN 2 L23
L24             1 E15-16 AND L23

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L29           926 L27 NOT L28
L30            84 C21H35N5
L31            20 L30 AND L27
L32            16 L31 AND NR>=4
L33             5 L32 AND (NC6 AND NCNC3 AND NC5 AND C6)/ES
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L37          32 L36 AND (PD<=20031209 OR AD<=20031209 OR PRD<=20031209)
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L39           1 L23 NOT L38
L40           1 L24 AND L27

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FILE 'REGISTRY' ENTERED AT 17:29:23 ON 19 FEB 2008
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STRUCTURE FILE UPDATES:   18 FEB 2008  HIGHEST RN 1004360-55-7
DICTIONARY FILE UPDATES:  18 FEB 2008  HIGHEST RN 1004360-55-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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L5              STR

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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT   2
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E6 C  E1 N  AT   1
ECOUNT  IS E4 C  E2 N  AT   2

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED    3911 ITERATIONS                          2301 ANSWERS
SEARCH TIME: 00.00.01



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FILE 'HCAPLUS' ENTERED AT 17:29:30 ON 19 FEB 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 19 Feb 2008 VOL 148 ISS 8
FILE LAST UPDATED: 18 Feb 2008 (20080218/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

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L22 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:383484 HCAPLUS
DN 144:428460
TI Method for measuring cell migration activity
IN Shibayama, Shiro; Takeda, Kazuhiko; Watanabe, Noriki; Sugiyama, Tetsuya
PA Ono Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2006043586	A1	20060427	2005WO-JP19187	20051019

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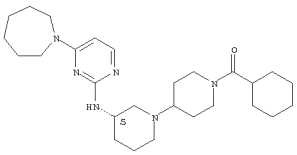
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI 2004JP-0305003 A 20041020

AB A method is provided for measuring the cell migration activity corresponding to the function of a specific cell migration inducer in vivo. The method comprises: (1) a process for transferring cells producing a cell migration inducer (e.g., MDC, SDF-1) into an air-pouch produced under a skin of a mammal (e.g., mouse) ; (2) a process for transferring cells to be measured (e.g., T cells, B cells, monocytes, macrophages, granulocytes) into a site other than the air-pouch of the mammal; (3) a process for recovering the cells in the air-pouch; and (4) a process for measuring the number of the cells to be measured in the recovered cells. Also provided are a method for evaluating a cell migration inhibitory compound possessing a specificity or a selectivity in vivo using the above method; and a method for producing the above cell migration inhibitory compound

IT 710981-61-6
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(method for measuring cell migration activity)
RN 710981-61-6 HCAPLUS
CN [1,4'-Bipiperidin]-3-amine, 1'-(cyclohexylcarbonyl)-N-[4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L22 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:515487 HCAPLUS

DN 141:71555

TI Preparation of nitrogen-containing heterocyclic compounds as CXCR4 regulators

IN Habashita, Hiromu; Kokubo, Masaya; Shibayama, Shiro; Tada, Hideaki; Tanihiro, Tatsuya

PA Ono Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 641 pp.
CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO2004052862	A1	20040624	2003WO-JP15718	20031209
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AU2003288994	A1	20040630	2003AU-0288994	20031209
EP----1571146	A1	20050907	2003EP-0778753	20031209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US2007167459	A1	20070719	2005US-0538758	20050610
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2003JP-0162706	A	20030606		
2003WO-JP15718	W	20031209		

OS MARPAT 141:71555

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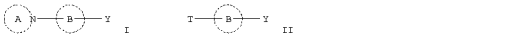

I II

AB Compds. such as pyrimidine and quinazoline derivs. represented by the following general formulas (I) and (II), salts thereof, N-oxides thereof, solvates thereof or prodrugs of the same (wherein the ring A represents an optionally substituted nitrogen-containing heterocycle; the ring B represents an optionally substituted homocycle or an optionally substituted heterocycle; Y represents an optionally substituted hydrocarbyl group, an optionally substituted heterocyclic group, an optionally protected amino group, an optionally protected hydroxyl group or an optionally protected mercapto group; and T represents the ring A or an optionally substituted amino group) are prepared. These compds. are CXCR4 regulators, in particular CXCR4 antagonists, and useful as preventives and/or remedies for various inflammatory diseases, immune diseases, various allergic diseases, infectious diseases, acquired immunodeficiency syndrome, infection with human immunodeficiency virus, psychiatric disorder, neurol. disease, cerebral diseases, cardiovascular diseases, metabolic diseases, or cancer, and agents for regeneration therapy, in particular transplant therapy. An assay system using SDF-1 which is an endogenous ligand of CXCR4 receptor, instead of HIV, was used in an assay for screening compds. which inhibit the binding of HIV to CXCR4 or CCR4 receptors on CD4-pos. cells. All the compds. prepared showed IC50 of 10 μM for inhibiting the binding of [125I]human SDF-1 to CEM cells, more specifically 0.1 μM for 2-(1-benzylpyrrolidin-3-ylamino)-4-(perhydroazepin-1-yl)pyrimidine. An ampule and tablet formulation containing 2-{[2-(dimethylamino)ethyl]amino}-4-(perhydroazepin-1-yl)pyrimidine were described.

IT 710978-26-0P 710978-30-6P 710978-41-9P
710978-46-4P 710978-49-7P 710978-55-5P
710978-59-9P 710978-64-6P 710978-70-4P

L22 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

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L22 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

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(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)

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(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)

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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
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(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists
for prepn. and/treatment of diseases)
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for prepn. and/treatment of diseases)
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L22 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
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(Uses)
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for prepn. and/treatment of diseases)
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
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(Uses)
(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists
for prepn. and/treatment of diseases)
IT 711002-73-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
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IT 710978-26-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
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(Uses)
(preparation of nitrogen-containing heterocyclic compds. as CXCR4 antagonists
for preparation and/treatment of diseases)
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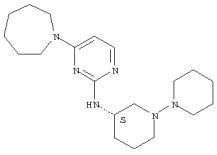
CN 2-Pyrimidinamine, N-(3S)-[1,1'-bipiperidin]-3-yl-4-(hexahydro-1H-azepin-1-
yl)- (CA INDEX NAME)

Absolute stereochemistry.

L22 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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L21 ANSWER 1 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:467883 HCAPLUS
DN 141:38627
TI Preparation of 2,4,6-trisubstituted pyrimidines as phosphatidylinositol (pi) 3-kinase inhibitors and their use in the treatment of cancer
IN Nuss, John M.; Pecchi, Sabina; Renhowe, Paul A.
PA Chiron Corporation, USA
SO PCT Int. Appl., 151 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

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PI WO2004048365	A1	20040610	2003WO-US37294	20031121 <--
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EP---1575940	A1	20050921	2003EP-0786980	20031121
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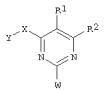

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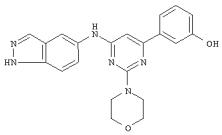
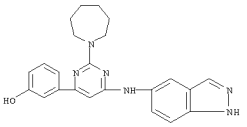


II

L21 ANSWER 1 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

AB Title compds. I [Y = (un)substituted alk(en/yn)yl, hetero/aryl, heterocyclyl; X = a direct link, NH and derivs., CH2 and derivs., O, S, SO, SO2, etc.; R1 = H, alkyl, CO2H, halo, OH and derivs., NH2 and derivs.; R2 = (un)substituted hetero/aryl, heterocyclyl; W = NH2 and derivs., (un)substituted alkyl, cyclyl containing at least one heteroatom; with provisos; their stereoisomers, tautomers, pharmaceutically acceptable salts, esters, or prodrugs] were prepared as phosphatidylinositol (pi) 3-kinase inhibitors for treating neoplasm. A solid phase synthesis is given for pyrimidine II•2CF3CO2H. Selected I displayed an IC50 < 20 μM in a cell proliferation assay.
IT 701243-14-3P, 3-{2-(Azepan-1-yl)-6-[(1H-indazol-5-yl)amino]pyrimidin-4-yl}phenol
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(phosphatidylinositol 3-kinase inhibitor; preparation of 2,4,6-trisubstituted pyrimidines as phosphatidylinositol 3-kinase inhibitors for treating neoplasm)
RN 701243-14-3 HCAPLUS
CN Phenol, 3-[2-(hexahydro-1H-azepin-1-yl)-6-(1H-indazol-5-ylamino)-4-pyrimidinyl]- (CA INDEX NAME)



RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:837052 HCAPLUS
DN 139:337980
TI Preparation of aminopyrimidines with muscarinic M3 antagonist and PDE IV inhibiting activity
IN Provins, Laurent; Van Keulen, Berend Jan; Surtees, John; Talaga, Patrice; Christophe, Bernard
PA UCB, S.A., Belg.
SO PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2003087064	A1	20031023	2003WO-EP03299	20030329 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU2003222786	A1	20031027	2003AU-0222786	20030329 <--
EP---1499598	A1	20050126	2003EP-0718717	20030329
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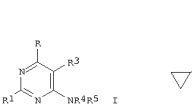
US2006074068	A1	20060406	2005US-0511660	20051005
PRAI 2002EP-0008706	A	20020418		
2003WO-EP03299	W	20030329		

OS MARPAT 139:337980
GI



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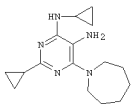
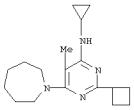


II

AB Aminopyrimidines I [R = NHR2, (un)substituted azetidinyl; R1 = alkyl, cycloalkyl; R2 = cycloalkyl; R3 = H, alkyl, halogen, OH, alkoxy, amino; R2R3 = alkylene; R4 = H, alkyl; R5 = cycloalkyl, aralkyl, heterocyclylalkyl; NR4R5 = heterocyclic], combining affinity and antagonism against the human M3 muscarinic receptor with activity as selective phosphodiesterase IV (PDE IV) inhibitors, were prepared. Thus, the amine II was prepared from 6-chloro-N,2-dicyclopropyl-5-nitropyrimidin-4-amine by reaction with hexamethylenimine and reduction of the nitro group.
IT 617716-91-3P 617716-94-6P 617716-96-8P
617717-01-8P 617717-03-0P 617717-04-1P
617717-05-2P 617717-06-3P 617717-08-5P
617717-10-9P 617717-12-1P 617717-13-2P
617718-39-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminopyrimidines with muscarinic M3 antagonist and PDE IV inhibiting activity)
RN 617716-91-3 HCAPLUS
CN 4-Pyrimidinamine, 2-cyclobutyl-N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
CRN 617716-90-2
CMF C18 H28 N4



CM 2

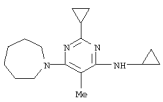
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 617716-94-6 HCAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617716-93-5
CMF C17 H26 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

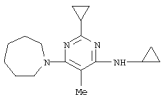
Double bond geometry as shown.

RN 617716-96-8 HCAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, (2E)-2-butenedioate (2:3) (CA INDEX NAME)

CM 1

CRN 617716-93-5
CMF C17 H26 N4

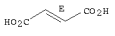
L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



CM 2

CRN 110-17-8
CMF C4 H4 O4

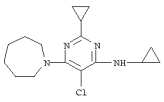
Double bond geometry as shown.



RN 617717-01-8 HCAPLUS
CN 4-Pyrimidinamine, 5-chloro-N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617717-00-7
CMF C16 H23 Cl N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

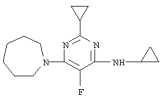
Double bond geometry as shown.

RN 617717-03-0 HCAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-5-fluoro-6-(hexahydro-1H-azepin-1-yl)-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617717-02-9
CMF C16 H23 F N4

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

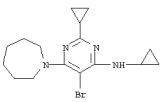


CM 2

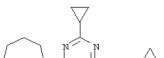
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

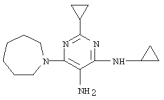
RN 617717-04-1 HCAPLUS
CN 4-Pyrimidinamine, 5-bromo-N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)



RN 617717-05-2 HCAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)



RN 617717-06-3 HCAPLUS
CN 4,5-Pyrimidinediamine, N4,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

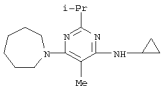


RN 617717-08-5 HCAPLUS

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-(1-methylethyl)-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617717-07-4
CMF C17 H28 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

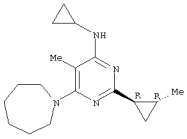
Double bond geometry as shown.

RN 617717-10-9 HCAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617717-09-6
CMF C18 H28 N4

Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

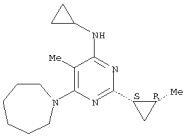
RN 617717-12-1 HCAPLUS

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-[(1R,2S)-2-methylcyclopropyl]-, rel-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617717-11-0
CMF C18 H28 N4

Relative stereochemistry.



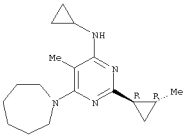
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

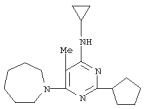
RN 617717-13-2 HCAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-(-)- (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



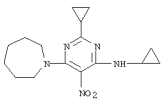
RN 617718-39-5 HCAPLUS
CN 4-Pyrimidinamine, 2-cyclopentyl-N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



● HCl

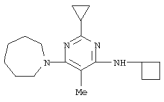
IT 617718-93-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aminopyrimidines with muscarinic M3 antagonist and PDE IV inhibiting activity)
RN 617718-93-1 HCAPLUS
CN 4-Pyrimidinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-nitro- (CA INDEX NAME)



IT 617716-99-1P 617717-14-3P 617717-16-5P
617717-17-6P 617717-18-7P 617718-28-2P
617718-57-7P 617718-60-2P 617718-71-5P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminopyrimidines with muscarinic M3 antagonist and PDE IV inhibiting activity)
RN 617716-99-1 HCAPLUS
CN 4-Pyrimidinamine, N-cyclobutyl-2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617716-98-0
CMF C18 H28 N4



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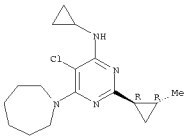
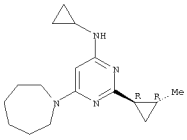
CRN 110-16-7
CMF C4 H4 O4

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

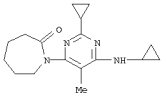


RN 617717-18-7 HCAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-2-[(1R,2R)-2-methylcyclopropyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 617718-28-2 HCAPLUS
CN 2H-Azepin-2-one, 1-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)

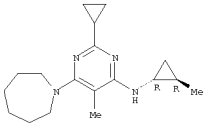


RN 617718-57-7 HCAPLUS
CN 4-Pyrimidinamine, 2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-N-[(1R,2R)-2-methylcyclopropyl]-, rel-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-56-6
CMF C18 H28 N4

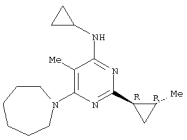
Relative stereochemistry.



L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
Double bond geometry as shown.

RN 617717-14-3 HCAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-(+)- (CA INDEX NAME)

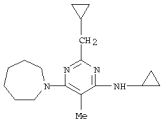
Rotation (+). Absolute stereochemistry unknown.



RN 617717-16-5 HCAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-2-(cyclopropylmethyl)-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617717-15-4
CMF C18 H28 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 617717-17-6 HCAPLUS
CN 4-Pyrimidinamine, 5-chloro-N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-2-[(1R,2R)-2-methylcyclopropyl]-, rel- (CA INDEX NAME)

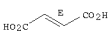
Relative stereochemistry.

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

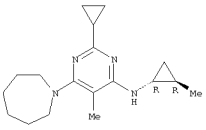


RN 617718-60-2 HCAPLUS
CN 4-Pyrimidinamine, 2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-N-[(1R,2R)-2-methylcyclopropyl]-, rel-, (2E)-2-butenedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-56-6
CMF C18 H28 N4

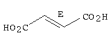
Relative stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

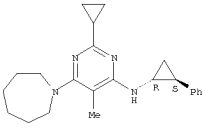


RN 617718-71-5 HCAPLUS
CN 4-Pyrimidinamine, 2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-N-[(1R,2S)-2-phenylcyclopropyl]-, rel-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-70-4
CMF C23 H30 N4

Relative stereochemistry.

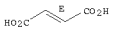


L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

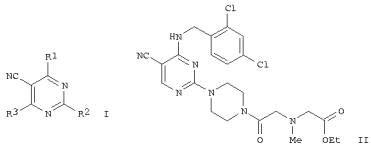


RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 3 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:796691 HCAPLUS
DN 139:307788
TI Preparation of 5-cyanopyrimidine derivatives as anti-inflammatory agents
IN Machii, Daisuke; Yamaura, Yosuke; Arai, Hitoshi; Yanagawa, Koji; Ohshima, Etsuo; Kawanabe, Ari; Iwase, Miho; Kobayashi, Katsuya; Sato, Takashi; Miki, Ichiro
PA Kyowa Hakko Kogyo Co., Ltd., Japan
SO PCT Int. Appl., 169 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

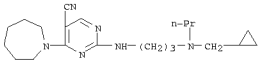
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2003082855	A1	20031009	2003WO-JP04009	20030328 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU2003220968	A1	20031013	2003AU-0220968	20030328 <--
PRAI 2002JP-0090640	A	20020328		
2003WO-JP04009	W	20030328		

OS MARPAT 139:307788
GI



AB The title pyrimidine compds. I [wherein R1 and R3 = independently H, OH, halo, (un)substituted alkyl, alkoxy, alkylthio, aryl, aralkyl, or amino; R2 = (un)substituted amino] or ammonium salts or pharmaceutically acceptable salts thereof are prepared as anti-inflammatory agents. For example, the compound II was prepared in a multi-step synthesis. II showed 97% inhibitory activity against thymus and activation-regulated chemokine (TARC) Hut78 cells at 1 μM. Formulations containing I as an active ingredient were also described.
IT 611202-14-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of cyanopyrimidine derivs. as anti-inflammatory agents)
RN 611202-14-3 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 2-[[3-[(cyclopropylmethyl)propylamino]propyl]amino]-4-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

L21 ANSWER 3 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

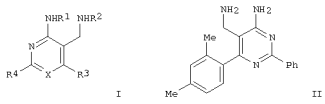


RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 4 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:656755 HCAPLUS
DN 139:197497
TI Preparation of novel pyridines and pyrimidines as DPP IV inhibitors
IN Boehringer, Markus; Loeffler, Bernd Michael; Peters, Jens-Uwe; Steger, Matthias; Weiss, Peter
PA F. Hoffmann-La Roche A.-G., Switz.
SO PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

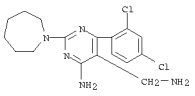
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2003068757	A1	20030821	2003WO-EP01107	20030205 <--
WO2003068757	A9	20041007		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA---2474578	A1	20030821	2003CA-2474578	20030205 <--
AU2003206833	A1	20030904	2003AU-0206833	20030205 <--
EP---1476435	A1	20041117	2003EP-0704536	20030205
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LI, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR2003007665	A	20050104	2003BR-0007665	20030205
CN---1630644	A	20050622	2003CN-0803774	20030205
JP2005526035	T	20050902	2003JP-0567888	20030205
RU----2293731	C2	20070220	2004RU-0127576	20030205
US2003216382	A1	20031120	2003US-0361268	20030210 <--
US---6867205	B2	20050315		
MX2004PA07744	A	20041015	2004MX-PA07744	20040810
US2005143405	A1	20050630	2005US-0037989	20050118
US---7022718	B2	20060404		
PRAI 2002EP-0003114	A	20020213		
2003WO-EP01107	W	20030205		
2003US-0361268	A3	20030210		

OS MARPAT 139:197497
GI



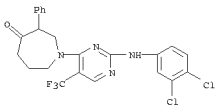
AB The title compds. [I; X = N, CR5; R1, R2 = H, alkyl; R3 = (un)substituted heterocyclyl or aryl; R4 = alkyl, alkoxy, alkylthio, etc.; R5 = H, alkyl], useful for the treatment and/or prophylaxis of diseases which are associated with DPP IV, such as diabetes, particularly non-insulin dependent diabetes mellitus, and impaired glucose tolerance, were prepared and formulated. Thus, reacting benzamidine with 2-(2,4-dimethylbenzylidene)malononitrile in the presence of K2CO3 in MeOH followed by treating the reaction residue with KMnO4 in Me2CO, and reduction of the resulting nitrile with LiAlH4 in THF afforded 7% II which showed IC50 of 0.172 μM against DPP IV.
IT 582306-20-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel pyridine and pyrimidine derivs. as DPP IV inhibitors)

L21 ANSWER 4 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RN 582306-20-5 HCAPLUS
CN 5-Pyrimidinemethanamine, 4-amino-6-(2,4-dichlorophenyl)-2-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

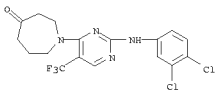


RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 5 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
R4 = (un)substituted alkyl; R5 = halo] and their pharmaceutically acceptable salts were prepd. For example, condensation of thiocyanatopyrimide II, e.g., prepd. from 3,4-dichloroaniline and 2-chloro-4-thiocyanato-5-nitropyrimidine in one step, and acetylaminoethylamine provided trisubstituted pyrimidine III in 88% yield. In CDK1/CyclinB1 kinase inhibition studies, 88-examples of compds. I exhibited IC50 values more than 100 nM. Compds. I are claimed useful for the treatment of diseases characterized by abnormal cell proliferation.
IT 514833-49-9P, 2-(3,4-Dichlorophenylamino]-4-(4-oxo-3-phenylazepan-1-yl)-5-trifluoromethylpyrimidine 514838-60-9P, 1-[2-(3,4-Dichlorophenylamino)-5-trifluoromethylpyrimidin-4-yl]azepan-4-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of trisubstituted pyrimidines as cyclin dependent kinase inhibitors)
RN 514833-49-9 HCAPLUS
CN 4H-Azepin-4-one, 1-[2-[(3,4-dichlorophenyl]amino]-5-(trifluoromethyl)-4-pyrimidinyl]hexahydro-3-phenyl- (CA INDEX NAME)



RN 514838-60-9 HCAPLUS
CN 4H-Azepin-4-one, 1-[2-[(3,4-dichlorophenyl]amino]-5-(trifluoromethyl)-4-pyrimidinyl]hexahydro- (CA INDEX NAME)

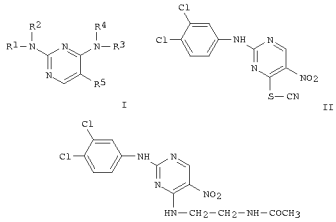


RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 5 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:319721 HCAPLUS
DN 138:321292
TI Preparation of 2,4,5-trisubstituted pyrimidines as cyclin dependent kinase inhibitors
IN Dahmann, Georg; Himmelsbach, Frank; Wittneben, Helmut; Pautsch, Alexander; Prokopowicz, Anthony S.; Krist, Bernd; Schnapp, Gisela; Steegmaier, Martin; Lenter, Martin; Schoop, Andreas; Steurer, Steffen; Spevak, Walter
PA Boehringer Ingelheim Pharma K.-G., Germany; Boehringer Ingelheim Pharmaceuticals, Inc.; Boehringer Ingelheim International G.m.b.H.
SO PCT Int. Appl., 278 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2003032997	A1	20030424	2002WO-EP11453	20021014 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA---2463989	A1	20030424	2002CA-2463989	20021014 <--
	AU2002340560	A1	20030428	2002AU-0340560	20021014 <--
	EP---1438053	A1	20040721	2002EP-0774710	20021014
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	JP2005509624	T	20050414	2003JP-0535800	20021014
	US2003171359	A1	20030911	2002US-0271763	20021016 <--
	US---7173028	B2	20070206		
	US2006100211	A1	20060511	2005US-0313380	20051221
PRAI	2001US-330145P	P	20011017		
	2002WO-EP11453	W	20021014		
	2002US-0271763	A3	20021016		

OS MARPAT 138:321292
GI



AB Title compds. I [R1 = H, alkyl; R2 = (un)substituted alkyl; R3 = H, alkyl;

L21 ANSWER 6 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2002:449449 HCAPLUS
DN 137:33318
TI Preparation of pyrimidinylaminothiazoles as tyrosine kinase inhibitors.
IN Bilodeau, Mark T.; Hartman, George D.; Hoffman, Jacob M., Jr.; Lumma, William C., Jr.; Manley, Peter J.; Rodman, Leonard; Sisko, John T.; Smith, Anthony M.; Tucker, Thomas J.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 169 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2002045652	A2	20020613	2001WO-US44573	20011130 <--
	WO2002045652	A3	20020822		
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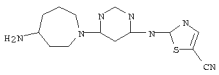
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US2002137755	A1	20020926	2001US-0990473	20011121 <--
	CA---2429728	A1	20020613	2001CA-2429728	20011130 <--
	AU2002032441	A	20020618	2002AU-0032441	20011130 <--
	EP---1341540	A2	20030910	2001EP-0991965	20011130 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP2004524282	T	20040812	2002JP-0547438	20011130
	US2004063720	A1	20040401	2003US-0677687	20031002 <--
	US---7115597	B2	20061003		
PRAI	2000US-251096P	P	20001204		
	2001US-0990473	A1	20011121		
	2001WO-US44573	W	20011130		

OS MARPAT 137:33318
GI

AB Title compds. [I; A, B = N, NO; Y = O, S, NR4; R1, R2 = H, perfluoroalkoxy, OH, cyano, halo, (substituted) alkyl(oxy)(carbonyl), aryl(oxy)(carbonyl), heterocyclyl, etc.; R4 = H, aryl, alkyl; R5 = H, SO2Rc, CORc, Rc, CO2Rc; R6 = aryl, cyano, halo, (substituted) alkyl, alkenyl, alkynyl, heterocyclyl, aminocarbonyl; Rc = alkyl, aryl, heterocyclyl], were prepared for treating angiogenesis, cancer, tumor growth, atherosclerosis, age related macular degeneration, diabetic retinopathy, inflammation, etc. Thus, 4-aminopyrimidine was stirred with NaH in THF; 2-bromo-5-phenylthiazole was added and the mixture was refluxed overnight to give 5-phenylthiazol-2-yl pyrimidin-4-yl amine. I inhibited vascular endothelial growth factor-stimulated mitogenesis of human vascular endothelial cells with IC50 = 0.01-5.0 nM.
IT 436851-15-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinylaminothiazoles as tyrosine kinase inhibitors)
RN 436851-15-9 HCAPLUS
CN 5-Thiazolecarbonitrile, 2-[[6-(4-aminohexahydro-1H-azepin-1-yl)-4-pyrimidinyl]amino]- (CA INDEX NAME)

L21 ANSWER 6 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

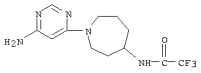


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

IT 436851-97-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidinylaminothiazoles as tyrosine kinase inhibitors)

RN 436851-97-7 HCAPLUS

CN Acetamide, N-[1-(6-amino-4-pyrimidinyl)hexahydro-1H-azepin-4-yl]-2,2,2-trifluoro- (CA INDEX NAME)

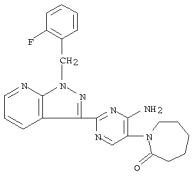


L21 ANSWER 7 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

IT 426818-40-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinyllactam-substituted pyrazolopyridines as inhibitors of cGMP degradation)

RN 426818-40-8 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-amino-2-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-5-pyrimidinyl]hexahydro- (CA INDEX NAME)



L21 ANSWER 7 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:391315 HCAPLUS

DN 136:386130

TI Preparation of pyrimidinyllactam-substituted pyrazolopyridines as inhibitors of cGMP degradation

IN Stasch, Johannes-Peter; Feurer, Achim; Weigand, Stefan; Stahl, Elke; Flubacher, Dietmar; Alonso-Alija, Cristina; Wunder, Frank; Lang, Dieter; Dembowsky, Klaus; Straub, Alexander; Perzborn, Elisabeth

PA Bayer AG, Germany

SO Ger. Offen., 38 pp.
CODEN: GWXXBX

DT Patent

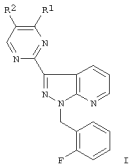
LA German

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE--10122895	A1	20020523	2001DE-1022895	20010511 <--
CA---2429308	A1	20020530	2001CA-2429308	20011109 <--
WO2002042299	A1	20020530	2001WO-EP12965	20011109 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU2002021827	A	20020603	2002AU-0021827	20011109 <--
EP---1339716	A1	20030903	2001EP-0997487	20011109 <--
EP---1339716	B1	20041103		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP2004520285	T	20040708	2002JP-0544433	20011109
ES---2231581	T3	20050516	2001ES-0997487	20011109
US---6903089	B1	20050607	2003US-0432740	20011109
PRAI 2000DE-1057752	A1	20001122		
2001DE-1022895	A	20010511		
2001WO-EP12965	W	20011109		

OS MARPAT 136:386130

GI



AB Title compds. [I; R1 = NH2, NHCO(C1-6 alkyl); R2 = R3NCOR4; R3NCOR4 = (substituted) (annelated) 5-7 membered heterocyclyl containing an addnl. heteroatom] were prepared Thus, an E/Z mixture of 3-(dimethylamino)-2-(3-oxo-4-morpholinyl)-2-propanenitrile (preparation given) was stirred with 1-(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridine-3-carboxamidine (preparation given) in xylene at 120° overnight to give 5.56% 4-(4-amino-2-(1-(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-5-pyrimidinyl)-3-morpholinone. Several I showed a vessel relaxation effect with IC50 = 0.25-1.99 μM.

L21 ANSWER 8 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 1998:542424 HCAPLUS

DN 129:245116

TI Novel antiallergic agents. Part I: synthesis and pharmacology of pyrimidine amide derivatives

AU Ban, Masakazu; Taguchi, Hiroaki; Katsushima, Takeo; Aoki, Shoichi; Watanabe, Akihiko

CS Pharmaceuticals Research Center, TOYOBO Co., Ltd., Shiga, 520-0292, Japan

SO Bioorganic & Medicinal Chemistry (1998), 6(7), 1057-1067
CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Science Ltd.

DT Journal

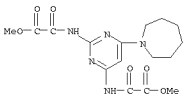
LA English

AB Pyrimidine amide derivs. were synthesized. Novel pyrimidine bis-glycolic amide derivs. showed moderate inhibition in the rat passive cutaneous anaphylaxis (PCA) assay by oral administration. Among these compds., 2,4-bis(methoxyacetylamino)-6-piperidinopyrimidine exhibited significant inhibition. However, 2,4-bis(methoxyacetylamino)-6-piperidinopyrimidine did not inhibit antigen-induced histamine or SRS-A release from lung fragments of the guinea-pig at less than 10-4 M. Derivs. of 2,4-bis(methoxyacetylamino)-6-piperidinopyrimidine have also notable or moderate activity in the rat PCA assay. An analog which has no oxygen atom at the α-position of the amide carbonyl group and a compound having no amide carbonyl group, showed no inhibition in the rat PCA assay. It was supposed that both the amide carbonyl group and the oxygen atom at α-position of the amide carbonyl group play an important role in inhibiting the rat PCA reaction. These pyrimidine bis-glycolic amide derivs. have a novel structure and unique activity which suggests they may be potentially useful in the treatment of allergic diseases.

IT 113259-20-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of pyrimidinyl amides as allergy inhibitors)

RN 113259-20-4 HCAPLUS

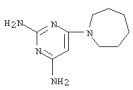
CN Acetic acid, 2,2'-[[6-(hexahydro-1H-azepin-1-yl)-2,4-pyrimidinediyl]diimino]bis[2-oxo-, dimethyl ester (9CI) (CA INDEX NAME)



IT 113259-25-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinyl amides as allergy inhibitors)

RN 113259-25-9 HCAPLUS

CN 2,4-Pyrimidinediamine, 6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

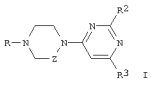


RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 9 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1997:377861 HCAPLUS
DN 126:343579
TI Preparation of pyrimidinylpiperazines as lipid peroxidation inhibitors
IN Toldy, Lajos; Zubovics, Zoltan; Szilagyi, Katalin; Vida, Franciska; Andrasi, Ferenc; Sutka, Klara; Hodula, Eszter; Szekeres, Tibor; Feher, Gabor; Moravcsik, Imre; Matyus, Peter; Sebestyen, Laszlo; Szabo, Hilda; Zara, Erzsebet; Horvath, Edit
PA Gyogyszerkutato Intezet, Hung.; Toldy, Marta; Toldy, Andras; et al.
SO PCT Int. Appl., 122 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

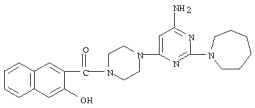
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO---9714685	A1	19970424	1996WO-HU00058	19961014 <--
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA				
HU-----76265	A2	19970728	1995HU-0003012	19951019 <--
AU---9673259	A	19970507	1996AU-0073259	19961014 <--
HU---9900088	A2	20000328	1999HU-0000088	19961014 <--
PRAI 1995HU-0003012	A	19951019		
1996WO-HU00058	W	19961014		

OS MARPAT 126:343579
GI

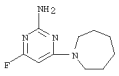


I

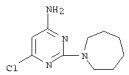
AB Title compds. [I; R = AX(CH2)r(CO)q(CH2)pR1; A = (un)substituted alkylene; R1 = (un)substituted aryl; R2,R3 = NH2 or N-attached heterocyclyl; X = bond, SO2, (un)substituted imino; Z = CH2 or CH2CH2; p,q,r = 0 or 1] were prepared Thus, 1-[2-hydroxy-3-(2-naphthylthio)propyl]piperazine (preparation given) was N-arylated by 2,6-diamino-4-chloropyrimidine to give I [R = R1SCH2CH(OH)CH2, R1 = 2-naphthyl, R2 = R3 = NH2, Z = CH2]. Data for biol. activity of I were given.
IT 190000-77-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinylpiperazines as lipid peroxidn. inhibitors)
RN 190000-77-2 HCAPLUS
CN Piperazine, 1-[6-amino-2-(hexahydro-1H-azepin-1-yl)-4-pyrimidinyl]-4-[(3-hydroxy-2-naphthalenyl)carbonyl]- (9CI) (CA INDEX NAME)



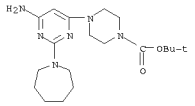
L21 ANSWER 10 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1997:266069 HCAPLUS
DN 126:277444
TI Synthesis and properties of 2,4-disubstituted 6-fluoropyrimidines
AU Popova, L. M.; Studentsov, E. P.
CS St. Petersburg. Gos. Tekhnol. Inst., St. Petersburg, 198013, Russia
SO Zhurnal Organicheskoi Khimii (1996), 32(9), 1424-1428
CODEN: ZORKAE; ISSN: 0514-7492
PB Nauka
DT Journal
LA Russian
OS CASREACT 126:277444
AB Reaction of 2,4,6-trifluoropyrimidine, 2-amino-4,6-difluoropyrimidine, and 4-amino-2,6-difluoropyrimidine with amines gave fluoropyrimidines containing two like or unlike amino groups.
IT 188987-82-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 188987-82-8 HCAPLUS
CN 2-Pyrimidinamine, 4-fluoro-6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)



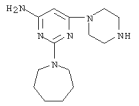
L21 ANSWER 9 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
IT 190001-49-1P 190001-50-4P 190001-51-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidinylpiperazines as lipid peroxidn. inhibitors)
RN 190001-49-1 HCAPLUS
CN 4-Pyrimidinamine, 6-chloro-2-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)



RN 190001-50-4 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[6-amino-2-(hexahydro-1H-azepin-1-yl)-4-pyrimidinyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



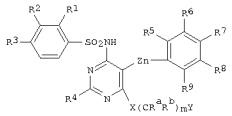
RN 190001-51-5 HCAPLUS
CN 4-Pyrimidinamine, 2-(hexahydro-1H-azepin-1-yl)-6-(1-piperazinyl)- (CA INDEX NAME)



L21 ANSWER 11 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1995:780258 HCAPLUS
DN 123:169647
TI Preparation of sulfonylaminopyrimidines as endothelin antagonists.
IN Breu, Volker; Burri, Kaspar; Cassal, Hean-Marie; Clozel, Martine; Hirth, Georges; Loeffler, Bernd-Michael; Mueller, Marcel; Neidhart, Werner; Ramuz, Henri
PA F. Hoffmann-La Roche AG, Switz.
SO Eur. Pat. Appl., 46 pp.
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP----633259	A1	19950111	1994EP-0109257	19940616 <--
EP----633259	B1	19990113		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
TW----394761	B	20000621	TW 1994-83105221	19940608 <--
CA---2125730	A1	19941229	1994CA-2125730	19940613 <--
CA---2125730	C	20051018		
AT----175669	T	19990115	1994AT-0109257	19940616 <--
ES---2127850	T3	19990501	1994ES-0109257	19940616 <--
ZA---9404434	A	19950103	1994ZA-0004434	19940621 <--
IL----110089	A	20000831	1994IL-0110089	19940622 <--
AU---9465948	A	19950105	1994AU-0065948	19940624 <--
AU----678467	B2	19970529		
HU-----67636	A2	19950428	1994HU-0001907	19940624 <--
FI---9403084	A	19941229	1994FI-0003084	19940627 <--
FI----112944	B1	20040213		
NO---9402428	A	19941229	1994NO-0002428	19940627 <--
NO----306403	B1	19991101		
BR---9402558	A	19950328	1994BR-0002558	19940627 <--
CN---1106007	A	19950802	1994CN-0106574	19940627 <--
CN---1050839	B	20000329		
LT-----3723	B	19960226	1994LT-0001979	19940627 <--
LV-----11175	B	19960620	1994LV-0000131	19940627 <--
US---5541186	A	19960730	1994US-0266072	19940627 <--
PL----175771	B1	19990226	1994PL-0304007	19940627 <--
PL----177031	B1	19990930	1994PL-0323036	19940627 <--
RU---2142457	C1	19991210	1994RU-0022258	19940627 <--
CZ----287184	B6	20001011	1994CZ-0001573	19940627 <--
JP--07017972	A	19950120	1994JP-0146003	19940628 <--
JP---2545200	B2	19961016		
RO----114325	B3	19990330	1994RO-0001112	19940628 <--
SK----280736	B6	20000711	1994SK-0000779	19940628 <--
PRAI 1993CH-0001924	A	19930628		
1992IL-0101650	A0	19920420		
1994CH-0001575	A	19940520		

OS MARPAT 123:169647
GI



I

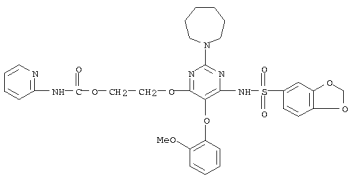
AB Title compds. (I; R1-R3 = H, alkyl, alkoxy, alkylthio, alkenyl, halo, CF3, hydroxyalkoxy, haloalkoxy, alkanoylalkyl, hydroxyalkyl, CO2H, amino, etc.; R2R3, R5R6, R6R7 = butadienyl, methylenedioxy, ethylenedioxy, isopropylidenedioxy; R4 = H, alkyl, cycloalkyl, CF3, alkoxy, alkynyloxy, alkylthio, alkylthioalkyl, hydroxyalkyl, dihydroxyalkoxy, alkylsulfinyl, alkylsulfonyl, aryl, arylthio, aryloxy, heterocyclyl, heterocyclylalkyl, etc.; R5-R9 = H, halo, CF3, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl; Ra, Rb = H, alkyl, alkoxy, alkylthio; X = O, S, NH; Y = O2CNR10R11, HNOCNR10R11, O2COR10, HNCO2R10; R10 = alkyl, cycloalkyl,

L21 ANSWER 11 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
hydroxyalkyl, carboxyalkyl, alkoxycarbonylalkyl, alkanoyloxyalkyl, arylcarbamoylalkyl, heterocyclyl, heterocyclylalkyl, etc.; R11 = H, R10; m = 1-3; n = 0,1), were prepd. Thus, 2-pyridinecarbonyl azide was heated in PhMe; 4-tert-butyl-N-[6-(2-hydroxyethoxy)-5-(2-methoxyphenoxy)-2,2'-bipyrimidin-4-yl]benzenesulfonamide was added to give pyridine-2-carbaminic acid, 2-[6-(4-tert-butylphenylsulfonylamino)-5-(2-methoxyphenoxy)-2,2'-bipyrimidin-4-yloxy]ethyl ester. The latter at 30 mg/kg orally in rats gave a 30% redn. in av. arterial blood pressure.

IT 167404-86-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of sulfonylaminopyrimidines as endothelin antagonists)

RN 167404-86-6 HCAPLUS

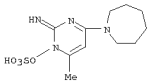
CN Carbamic acid, 2-pyridinyl-, 2-[[6-[(1,3-benzodioxol-5-ylsulfonyl)amino]-2-(hexahydro-1H-azepin-1-yl)-5-(2-methoxyphenoxy)-4-pyrimidinyl]oxy]ethyl ester (9CI) (CA INDEX NAME)



L21 ANSWER 12 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 137216-16-1 HCAPLUS

CN 2(1H)-Pyrimidinimine, 4-(hexahydro-1H-azepin-1-yl)-6-methyl-1-(sulfooxy)- (CA INDEX NAME)



L21 ANSWER 12 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 1991:656199 HCAPLUS

DN 115:256199

TI Preparation of N-sulfoxypyrimidine inner salts and pyrimidine N-oxides as hair loss retardants

IN Dufetel, Didier; Estradier, Francoise; Gaetani, Quintino; Hocquaux, Michel

PA Fr.

SO Can. Pat. Appl., 83 pp.
CODEN: CPXXEB

DT Patent

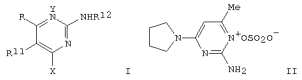
LA French

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA---2024156	A1	19910301	1990CA-2024156	19900828 <--
CA---2024156	C	20020101		
FR---2651122	A1	19910301	1989FR-0011352	19890829 <--
FR---2651122	B1	19941028		
EP----420707	A1	19910403	1990EP-0402361	19900824 <--
EP----420707	B1	19931215		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE				
AT----98468	T	19940115	1990AT-0402361	19900824 <--
JP--03118372	A	19910520	1990JP-0224531	19900828 <--
JP---3053200	B2	20000619		
CA---2285886	C	20020101	1990CA-2285886	19900828 <--
US---5610302	A	19970311	1995US-0461848	19950605 <--
US---5760043	A	19980602	1996US-0768533	19961218 <--
PRAI 1989FR-0011352	A	19890829		
1990EP-0402361	A	19900824		
1990US-0573578	B1	19900827		
1990CA-2024156	A3	19900828		
1994US-0224176	A3	19940407		

OS MARPAT 115:256199

GI

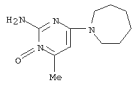


AB Title compds. [I; R = H, alkyl; R11 = H; RR11 = (CH2)3-5; R12 = H, alkanoyl, alkoxycarbonyl, substituted CONH2; X = H, NR1R2, alkoxy, alkylthio, PhO, etc.; R1, R2 = H, (cyclo)alkyl, alkenyl, (un)substituted Ph, etc.; NR1R2 = heterocyclyl; Y = O, OSO3- (N has pos. charge)] were prepared as hair loss retardants (no data). Thus, 2-amino-4-methyl-6-chloropyrimidine N-oxide was condensed with pyrrolidine and the product treated with pyridine-SO3 complex to give title compound II.

IT 137216-12-7P 137216-16-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as hair loss retardant and growth stimulant)

RN 137216-12-7 HCAPLUS

CN 2-Pyrimidinamine, 4-(hexahydro-1H-azepin-1-yl)-6-methyl-, 1-oxide (CA INDEX NAME)



L21 ANSWER 13 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 1991:559166 HCAPLUS

DN 115:159166

TI Preparation of pyrimidinium derivatives as cardiovascular agents

IN Hargreaves, Rodney Brian; McLouchlin, Bernard Joseph; Mills, Stuart Dennett

PA Imperial Chemical Industries PLC, UK

SO Eur. Pat. Appl., 31 pp.
CODEN: EPXXDW

DT Patent

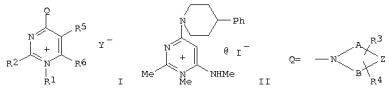
LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP----434341	A1	19910626	1990EP-0313772	19901217 <--
EP----434341	B1	19950517		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU-----56087	A2	19910729	1990HU-0008115	19901207 <--
HU-----207511	B	19930428		
ZA----9009852	A	19911030	1990ZA-0009852	19901207 <--
AU---9067914	A	19910627	1990AU-0067914	19901210 <--
AU----641960	B2	19931007		
NO---9005378	A	19910624	1990NO-0005378	19901212 <--
ES---2072993	T3	19950801	1990ES-0313772	19901217 <--
US---5252567	A	19931012	1990US-0629502	19901218 <--
CA---2032743	A1	19910623	1990CA-2032743	19901219 <--
FI---9006306	A	19910623	1990FI-0006306	19901220 <--
JP--03291277	A	19911220	1990JP-0404924	19901221 <--
PRAI 1989GB-0029022	A	19891222		

OS MARPAT 115:159166

GI

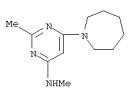


AB Title compds. I [R1 = C1-10 alkyl, C3-8 cycloalkyl, (substituted) Ph, etc.; R2 = H, C1-4 alkyl, H2N, C1-4 alkylamino; R5 = H, C1-4 alkyl, C2-4 alkenyl; R6 = C1-4 alkyl, H2N, C1-4 alkylamino; R3, R4 = H, C1-4 alkyl, (substituted) Ph, PhCH2; A, B = CH2CH2, (CH2)3; Z = bond, O, S, CO, CH2, etc.; Y = amino], are prepared 2-Methyl-6-(methylamino)-4-(4-phenylpiperidino)pyrimidine (preparation given) and MeI in dioxane were refluxed for 15 h to give the piperidinium II. II had an IC20 of 10-6M as a bradycardic effect (reduction in beating rate of spontaneously beating isolated pig right atrium). A capsule and tablet formulation comprising I are given.

IT 136346-61-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and quaternization of, with Me iodide)

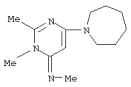
RN 136346-61-7 HCAPLUS

CN 4-Pyrimidinamine, 6-(hexahydro-1H-azepin-1-yl)-N,2-dimethyl- (CA INDEX NAME)



IT 136346-34-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU

L21 ANSWER 13 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as cardiovascular agent)
RN 136346-34-4 HCAPLUS
CN Methanamine, N-[6-(hexahydro-1H-azepin-1-yl)-2,3-dimethyl-4(3H)-pyrimidinylidene]-, monohydriodide (9CI) (CA INDEX NAME)

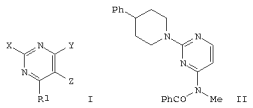


● HI

L21 ANSWER 14 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1991:23983 HCAPLUS
DN 114:23983
TI Preparation of 2-aminopyrimidines as nervous system agents
IN Tomino, Ikuo; Takesue, Mitsuyuki; Kihara, Noriaki; Kitahara, Takumi; Awaya, Akira; Horikomi, Kazutoshi; Sasaki, Tadayuki; Mizuchi, Akira
PA Mitsui Petrochemical Industries, Ltd., Japan; Mitsui Pharmaceuticals, Inc.
SO Eur. Pat. Appl., 154 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

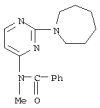
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP----379806	A2	19900801	1989EP-0313595	19891227 <--
	EP----379806	A3	19910529		
	EP----379806	B1	19960410		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP--02221275	A	19900904	1989JP-0041729	19890223 <--
	HU-----52769	A2	19900828	1989HU-0006762	19891222 <--
	HU----206337	B	19921028		
	HU-----61293	A2	19921228	1992HU-0001485	19891222 <--
	HU----210001	B	19950130		
	HU-----61313	A2	19921228	1992HU-0001487	19891222 <--
	HU----209594	B	19940829		
	HU-----61288	A2	19921228	1992HU-0001488	19891222 <--
	HU----209574	B	19940829		
	JP--03014568	A	19910123	1989JP-0334759	19891226 <--
	JP---2744663	B2	19980428		
	EP----612746	A1	19940831	1994EP-0105018	19891227 <--
	R: DE, FR, GB, IT				
	AT----136542	T	19960415	1989AT-0313595	19891227 <--
	AU---8947329	A	19900705	1989AU-0047329	19891228 <--
	AU----629595	B2	19921008		
	CA---2006944	A1	19900629	1989CA-2006944	19891229 <--
	CN---1045390	A	19900919	1989CN-0109731	19891229 <--
	CN---1037513	B	19980225		
	US---5147876	A	19920915	1989US-0459376	19891229 <--
	US---5264435	A	19931123	1992US-0888726	19920526 <--
	CN---1090846	A	19940817	1993CN-0119388	19931021 <--
PRAI	1988JP-0333670	A	19881229		
	1989JP-0041728	A	19890223		
	1989JP-0041729	A	19890223		
	1989HU-0006762	A3	19891222		
	1989EP-0313595	A3	19891227		
	1989US-0459376	A3	19891229		

OS MARPAT 114:23983
GI

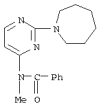


AB The title compds. [I; R1 = H, alkyl; X = morpholino, (substituted) pyrrolidino, piperidino, azepino, piperazino, tetrahydroquinolinyl, tetrahydroisoquinolinyl, etc.; Y = amino, pyridin-4-ylcarbonyl, piperidinyl-N-carbonyl, phenylcarbamoyl, benzoyl, phthalimido, etc., CH2R2; R2 = H, alkyl, alkoxy, alkylthio, dialkylamino; Z = H, halo, alkyl, alkoxycarbonyl], were prepared Thus MeNH2 in MeOH was added to 2,4-dichloropyrimidine in CH2Cl2 at 5° followed by stirring for 12 h at room temperature to give 2-chloro-4-methylaminopyrimidine. The latter was heated with 4-phenylpiperidine in BuOH at 130° for 1 h to give

L21 ANSWER 14 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
4-methylamino-2-(4-phenylpiperdino)pyrimidine. The latter in THF contg. Et3N was treated with PhCOCl in THF and then with pyridine. The mixt. was stirred 2 days to give 70% title compd. II. I increased twitch tension in rats with crushed sciatic nerves from 33.3% of normal (controls) to 48.1-51.2% at 10-30 ng/kg i.p. daily over 30 d.
IT 131037-57-5P 131038-83-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as nervous system agent)
RN 131037-57-5 HCAPLUS
CN Benzamide, N-[2-(hexahydro-1H-azepin-1-yl)-4-pyrimidinyl]-N-methyl- (CA INDEX NAME)

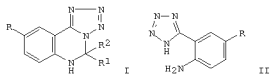


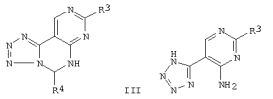
RN 131038-83-0 HCAPLUS
CN Benzamide, N-[2-(hexahydro-1H-azepin-1-yl)-4-pyrimidinyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

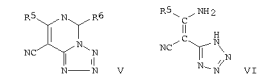


● HCl

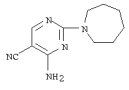
L21 ANSWER 15 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1988:590353 HCAPLUS
DN 109:190353
TI Synthesis of new substituted 5,6-dihydrotetrazolo[1,5-c]quinazolines, tetrazolo[1,5-c]quinazolines, 5,6-dihydropyrimido[5,4-e]tetrazolo[1,5-c]pyrimidines, and 5,6-dihydrotetrazolo[1,5-c]pyrimidines
AU Ried, Walter; Aboul-Fetouh, Saleh
CS Inst. Org. Chem., Univ. Frankfurt, Frankfurt/Main, D-6000/70, Fed. Rep. Ger.
SO Chemiker-Zeitung (1988), 112(4), 135-40
CODEN: CMKZAT; ISSN: 0009-2894
DT Journal
LA German
OS CASREACT 109:190353
GI



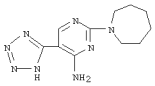




AB 5,6-Dihydrotetrazolo[1,5-c]quinazolines I [R = H, Cl, O2N; R1 = CCl3, C6H2(OMe)3-3,4,5, C6H4CO2Me-4, C6H3Cl2-2,6, C6H4Cl-4; R2 = H] were prepared by cyclocondensation of tetrazolylanilines II with R1CHO. I (R = H, Cl, O2N; R1 = Me, Pr; R2 = Et, Pr, COMe, CH2COMe) were prepared by cyclocondensation of II with R1COR2. 5,6-Dihydropyrimido[5,4-e]tetrazolo[1,5-c]pyrimidines III [R3 = SEt, pyrrolidino, piperidino, morpholino, hexahydro-1H-azepin-1-yl; R4 = Ph, C6H4CO2Me-4, C6H3Cl2-2,6, C6H4Cl-4, C6H4NO2-4, C6H2(OMe)3-3,4,5, C6H4NO2-2] were prepared by cyclocondensation of aminotetrazolylpyrimidines IV with R4CHO. 5,6-Dihydrotetrazolo[1,5-c]pyrimidines V [R5 = H, Me, MeS; R6 = Ph, C6H3Cl2-2,6, C6H4CO2Me-4, C6H2(OMe)3-3,4,5, C6H4Cl-2] were prepared from nitriles VI and R6CHO.
IT 117086-03-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with azide, tetrazole derivative from)
RN 117086-03-0 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 4-amino-2-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)



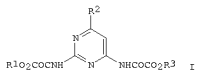
L21 ANSWER 15 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
IT 117085-75-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with aldehydes)
RN 117085-75-3 HCAPLUS
CN 4-Pyrimidinamine, 2-(hexahydro-1H-azepin-1-yl)-5-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



L21 ANSWER 16 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1988:112484 HCAPLUS
DN 108:112484
TI Preparation of heterocyclylpyrimidinedioxamates as allergy inhibitors
IN Taguchi, Hiroaki; Katsushima, Takeo; Ban, Masakazu; Aoki, Shoichi; Watanabe, Akihiko
PA Toyobo Co., Ltd., Japan
SO Eur. Pat. Appl., 21 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

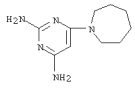
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP----243817	A1	19871104	1987EP-0105671	19870416 <--
R: DE, FR, IT				
US----4729995	A	19880308	1987US-0033734	19870403 <--
JP--63246368	A	19881013	1987JP-0091615	19870414 <--
PRAI 1986JP-0091482	A	19860421		
1986JP-0279040	A	19861122		

OS CASREACT 108:112484; MARPAT 108:112484
GI



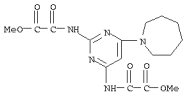
I

AB The title compds. [I; R1, R3 = H, alkyl, PhCH2, alkali metal cation, NH4+; R2 = H, halo, alkyl, alkoxy, aryl, NH2, (hetero)cyclic amino] were prepared as allergy inhibitors. 2,4-Diamino-6-piperidinopyrimidine in pyridine was condensed with Et oxalyl chloride with initial cooling. The mixture was worked up after 1 h at room temperature to give I (R1 = R3 = Et, R2 = piperidino) (II). At 3 mg/kg i.v. in rats, II gave 90.6% inhibition of passive cutaneous anaphylaxis.
IT 113259-25-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, by alkyl oxalyl chloride, in preparation of allergy inhibitor)
RN 113259-25-9 HCAPLUS
CN 2,4-Pyrimidinediamine, 6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

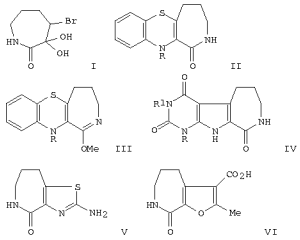


IT 113259-20-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as allergy inhibitor)
RN 113259-20-4 HCAPLUS
CN Acetic acid, 2,2'-[[6-(hexahydro-1H-azepin-1-yl)-2,4-pyrimidinediyl]diimino]bis[2-oxo-, dimethyl ester (9CI) (CA INDEX NAME)

L21 ANSWER 16 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

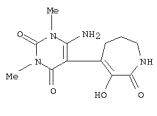


L21 ANSWER 17 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1978:443306 HCAPLUS
DN 89:43306
ORER 89:6729a,6732a
TI Study of lactams. XXIX. Synthesis and some reactions of 2-oxo-3,3-dihydroxy-4-bromohexahydroazepine
AU Glushkov, R. G.; Smirnova, V. G.; Zasosova, I. M.; Stezhko, T. V.; Ovcharova, I. M.; Vlasova, I. F.
CS Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1978), (3), 374-8
CODEN: KGSSAQ; ISSN: 0453-8234
DT Journal
LA Russian
OS CASREACT 89:43306
GI



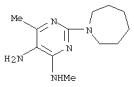
I II III IV V VI

AB Condensation of the title compound I with o-RNHC6H4SH gave 23-77% II (R = H, Et, PhCH2, Me2NCH2CH2, Et2NCH2CH2). Treatment with Et3O+BF4- gave 37 and 49% III (R = Et, PhCH2). Pyrimidopyrroloazepines IV (R = Me, H, R1 = Me; R = Me, R1 = H) were obtained in 4-50% yields by condensation of I with the corresponding aminouracils. Condensation of I with thiourea gave 75% V and condensation with MeCOCH2CO2Et gave 40% VI.
IT 66751-44-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 66751-44-8 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 6-amino-1,3-dimethyl-5-(2,5,6,7-tetrahydro-3-hydroxy-2-oxo-1H-azepin-4-yl)-, monohydrobromide (9CI) (CA INDEX NAME)

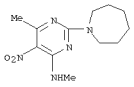


● HBr

L21 ANSWER 18 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1976:17283 HCAPLUS
DN 84:17283
OREF 84:2863a,2866a
TI Purine studies. XVII. Synthesis of 2-substituted 6,9-di- and 6,8,9-trimethylpurines as amplifiers of phleomycin
AU Bhushan, Kul; Brown, Desmond J.; Lister, John H.; Stephanson, Lawrence G.; Yoneda, Fumio
CS John Curtin Sch. Med. Res., Canberra, Australia
SO Australian Journal of Chemistry (1975), 28(11), 2553-9
CODEN: AJCHAS; ISSN: 0004-9425
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB 2-(6,8,9-Trimethylpurin-2-ylthio)acetamide (I, R = SCH2CONH2, R1 = Me) and analogous N-substituted acetamides are prepared by treatment of 6,8,9-trimethylpurine-2-thione with an appropriate 2-chloroacetamide. 6,9-Dimethyl-2-(piperidin-1-yl)purine I(R = piperidino, R1 = H) and some 2-polymethyleneamino homologues are made by initial amination of 2-chloro-4-methyl-6-methylamino-5-nitropyrimidine followed by reduction of the nitro group and final cyclization with HCO2H. Such purines enhance the lethal effect of phleomycin on Escherichia coli cultures.
IT 57880-52-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, purine derivs. from)
RN 57880-52-1 HCAPLUS
CN 4,5-Pyrimidinediamine, 2-(hexahydro-1H-azepin-1-yl)-N4,6-dimethyl- (CA INDEX NAME)



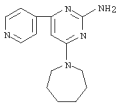
IT 57880-51-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 57880-51-0 HCAPLUS
CN 4-Pyrimidinamine, 2-(hexahydro-1H-azepin-1-yl)-N,6-dimethyl-5-nitro- (CA INDEX NAME)



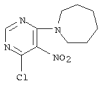
L21 ANSWER 19 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1975:140173 HCAPLUS
DN 82:140173
OREF 82:22399a,22402a
TI 2,4,6-Trisubstituted pyrimidines
IN Tani, Hideo; Nakamura, Koji; Mori, Shizuhiro; Yokoo, Nobuo; Kyotani, Yoshitoku; Wada, Yasushi
PA Kowa Co., Ltd.
SO Jpn. Tokkyo Koho, 12 pp.
CODEN: JAXXAD
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP--49021148	B	19740530	1970JP-0127609	19701228 <--
PRAI 1970JP-0127609		19701228		

GI For diagram(s), see printed CA Issue.
AB Sixty-three antiinflammatory (no data) pyrimidines (R = 4-pyridyl, Ph, etc., R1 = NH2, NMe2, NEt2, morpholino, NHPr, piperidino, OMe, etc., R2 = NMe2, OCH2CH2NMe2, NEt2, morpholino, NHCH2CH:CH2, NHCH2CH2OH, etc.) were prepared by reacting I (R1 = SO2Me or Cl) with the appropriate amine or alc. E.g., I (R = NH2, R1 = SO2Me, R2 = 4-pyridyl) (0.016 mole) was refluxed 1 hr with 30 ml MeOH containing 0.03 mole Na to give 80% I (R = NH2, R1 = OMe, R2 = 4-pyridyl).
IT 54993-89-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54993-89-4 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-1H-azepin-1-yl)-6-(4-pyridinyl)- (CA INDEX NAME)



L21 ANSWER 20 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1975:4203 HCAPLUS
DN 82:4203
OREF 82:727a,730a
TI Heterocyclic studies. XXXI. New routes to reduced imidazole, pyrimidine, and pyridopyrimidine derivatives
AU Clark, Jim; Curphey, Michael; Southon, Ian W.
CS Ramage Lab., Univ. Salford, Salford, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1974), (14), 1611-14
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB Six 4-(substituted amino)-6-chloro-5-nitropyrimidines [I, e.g. R = NEtPh, NH(CH2)2OH] with dilute AcOH gave RC(NH2):C(CN)NO2. I [R = NMe(CH2)2OH] with POCl3 followed by H2O gave the reduced imidazole II (R = Me) via the quaternary salt III. Similarly I [R = N[(CH2)2Cl]2] gave II [R = (CH2)2Cl] and I [R = NPh(CH2)3OH] gave the hexahydropyrimidines IV (R = H and CHO), and 4-chloro-6-[2-(2-hydroxyethyl)piperidino]-2-methyl-5-nitropyrimidine gave the pyridopyrimidine V.
IT 54413-32-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring cleavage of)
RN 54413-32-0 HCAPLUS
CN 1H-Azepine, 1-(6-chloro-5-nitro-4-pyrimidinyl)hexahydro- (CA INDEX NAME)

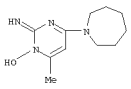


L21 ANSWER 21 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1969:115172 HCAPLUS
DN 70:115172
OREF 70:21518h,21519a
TI 1,2-Dihydro-1-hydroxy-2-imino-6-methyl-4-(dialkylamino)pyrimidines and 1,6-dihydro-1-hydroxy-6-imino-2-methyl-4-(dialkylamino)pyrimidines
IN Ursprung, Joseph J.; Anthony, William C.
PA Upjohn Co.
SO Fr., 38 pp.
CODEN: FRXXAK
DT Patent
LA French
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI FR---1513739	A1	19680216	1967FR-0095687	19670220 <--
PRAI 1966US-0528790	A	19660221		

OS MARPAT 70:115172
GI For diagram(s), see printed CA Issue.
AB 2-Amino-6-methyl-4-(R-substituted)-5-(R1-substituted)-pyrimidines (I) and 6-amino-2-methyl-4-(R-substituted)-5-(R1-substituted)-pyrimidines (II), where R is an aryloxy group, are treated with HOOAc and m-ClC6H4C(O)OOH to give 1,2-dihydro-1-hydroxy-2-imino-4-(R-substituted)-5-(R1-substituted)-pyrimidines (III) and 1,6-dihydro-1-hydroxy-6-imino-4-(R-substituted)-5-(R1-substituted)-pyrimidines (IV). III and IV, where R is an aryloxy group, are treated with amines to give 4-amino compds. Thus, 28.6 g. I (R = Cl, R1 = H) is treated with 94 g. PhOH in the presence of KOH at 95-100° to give 79% 2-amino-6-methyl-4-phenoxypyrimidine (V), m. 192-4°. A solution of 14.2 g. V and 0.14 mole HOOAc in 150 ml. HOAc is heated 20 hrs. at 58° to give 28% 1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-phenoxypyrimidine (VI), m. 190-3°. VI (1.0 g.) is added to a solution of 0.96 g. Na and 0.005 g. FeCl3 in 20 ml. piperidine, and the mixture refluxed 2 hrs. to give 41% 1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-piperidinopyrimidine. Similarly prepared are I (R = 2,4-Cl2C6H3O, R1 = H), m. 195-6°; I = (R = 2,4-Cl2C6H3O, R1 = Me), m. 157-8°; the following III (R, R1, and m.p. given): 2,4-Cl2C6H3O, H, 216-18°; piperidino, H, 260-1°; pyrrolidino, H, 271-3°; morpholino, H, 261° (decompose 264-7°); 4-methyl-1-piperazinyl, H, 212-13° (2,4-Cl2C6H3OH salt m. 151-2°); hexamethylenimino, H, 208-10°; Me2N, H, 228-9°; CH2:CHCH2NH, H, 252-5° (decomposition); PhCH2NH, H, 227-9°; 2,4-Cl2C6H3O, Me, 225-6°; piperidino, Me, 172-3°; 2,4-Cl2C6H3O, Br, 212-14°; pyrrolidino, Br, 166-7°; II (R = 2,4-Cl2C6H3O, R1 = H), m. 157-8°; and the following IV (R, R1, and m.p. given): 2,4-Cl2C6H3O, H, 214-16°; piperidino, H, 200-200.5°; 2,4-Cl2C6H3O, Br, -; pyrrolidino, Br, -. III (R1 = Br) and IV (R1 = Br) are treated with amines and thiophenols to give the following III (R, R1, and m.p. given): pyrrolidino, pyrrolidino, 224-6°; pyrrolidino, piperidino, - (monohydrate m. 204-6°); pyrrolidino, p-ClC6H4S, 169-70°; and the following compds.: IV (R = R1 = pyrrolidino), IV (R = pyrrolidino, R1 = p-ClC6H4S). A mixture of 5.4 g. III (R = pyrrolidino, R1 = Br) and 50 ml. pyrrolidine is heated 3 hrs. at 108-10° to give III (R = pyrrolidino, R1 = H) and III (R = R1 = pyrrolidino), m. 186-7°, in a 1:1 weight ratio. Also prepared, according to known methods (halogenation, nitration, NO2 group reduction, acylation), are the following compds. (m.p. given): I (R = 2,4-Cl2C6H3O, R1 = Br), 155-6.5°; III (R = piperidino, R1 = NO2), 196-9°; III (R = piperidino, R1 = NH2), -; II (R = 2,4-Cl2C6H3O, R1 = Br), -; IV (R = piperidino, R1 = NO2), -; IV (R = piperidino, R1 = NH2), -; III (R = piperidino, R1 = H).HCl, -; and 1,2-dihydro-1-hydroxy-2-acetylimino-6-methyl-4-piperidinopyrimidine, -. Uv and ir data are given. (In this abstract, pyrrolidino-1-pyrrolidinyl.)
IT 22370-34-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 22370-34-9 HCAPLUS
CN 1H-Azepine, 1-(1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-pyrimidinyl)hexahydro- (8CI) (CA INDEX NAME)

L21 ANSWER 21 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

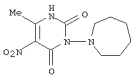


L21 ANSWER 22 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1967:454154 HCAPLUS
DN 67:54154
OREF 67:10195a,10198a
TI Uracils in herbicide compositions
IN Loux, Harvey M.
PA du Pont de Nemours, E. I., and Co.
SO Fr., 21 pp.
CODEN: FRXXAK
DT Patent
LA French
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI FR---1461796		19661209	FR	<--
CH----480013			CH	
DE---1567038			DE	
GB---1115786			GB	
PRAI US		19641207		

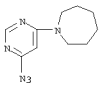
AB 6-Methyluracil derivs. were prepared and used in herbicidal compns. Thus, a mixture of 1-(hexahydro-1-azepinyl)urea 126, Et acetoacetate 104, p-MeC6H4SO3H 4, and PhMe 1300 parts was heated under reflux 20 hrs. A 29% NaOMe-MeOH solution (200 parts) was added to the cooled solution, and heating continued 3 hrs. The mixture was cooled, shaken with ice (1000 parts), separated, and the organic layer shaken with H2O. The combined aqueous layers were washed with CH2Cl2. Acidification of the aqueous layers precipitated 3-(hexahydro-1-azepinyl)-6-methyluracil (I). Cl (8 parts) was added to a solution of 22.3 parts I and 16 parts anhydrous NaOAc in 100 parts HOAc at 30°. The solution was shaken for a further 30 min. and poured into H2O (200 parts) to precipitate 5-chloro-3-(hexahydro-1-azepinyl)-6-methyluracil. Also prepared from I were the following 3-(hexahydro-1-azepinyl)-6-methyluracils (substituents given): 5-(hydroxymethyl)-5-nitro, 5-iodo, 5-(methoxymethyl), 1-methyl. Also prepared was 3-(hexahydro-1-azepinyl)-6-methyl-4-thiouracil. Other compds. claimed were: 5-bromo-6-methyl-3-(1-piperidino)uracil; 5-chloro-6-methyl-3-(1-piperidino)uracil; 5-bromo-6-methyl-3-(pyrrolidinyl)uracil; 5-chloro-6-methyl-3-(1-pyrrolidinyl)uracil; 5-bromo-6-methyl-3-(hexahydro-1-azepinyl)uracil; 5-bromo-6-methyl-3-(4-morpholino)uracil.

IT 14785-91-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14785-91-2 HCAPLUS
CN Uracil, 3-(hexahydro-1H-azepin-1-yl)-6-methyl-5-nitro- (8CI) (CA INDEX NAME)

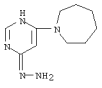


L21 ANSWER 23 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1966:93457 HCAPLUS
DN 64:93457
OREF 64:17589g-h,17590a
TI Tetrazole-azidoazomethine rearrangements in pyrimidine series
AU Postovskii, I. Ya.; Smirnova, N. B.
CS S. M. Kirov Polytech. Inst., Sverdlovsk
SO Doklady Akademii Nauk SSSR (1966), 166(5), 1136-9
CODEN: DANKAS; ISSN: 0002-3264
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB Addition of N2H4.H2O to 4,6-dichloropyrimidine in MeOH (exothermic) rapidly gave 66% 4-hydrazino-6-chloropyrimidine, m. 164-5°, which heated with aqueous amines 2 hrs. gave 65-70% 4-hydrazino-6-substituted-pyrimidines (substituent shown): morpholino, m. 166-7°; N-homopiperidinyl, m. 126-7°; N-pyrrolidinyl, m. 195-6°; piperidino, m. 122-3°. These treated with 2N HCl, followed by aqueous NaNO2 at 0°, gave 80-95% 4-azido-6-substituted-pyrimidines: morpholino, m. 92-3°; N-homopiperidinyl, m. 52°. The remaining enos were converted by this reaction into tetrazolo[c]-7-substituted-pyrimidines (I): N-pyrrolidinyl, m. 97°; piperidino, m. 77-8°. Ir spectra are shown. Thus, the presence of only electron-donor substituents leads to linear and cyclic nitrosation products. The tetrazole structures existed only in the solid state in the above products; in solution these were equilibrated with the azides (II), as shown spectroscopically

IT 5767-40-8
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 5767-40-8 HCAPLUS
CN 1H-Azepine, 1-(6-azido-4-pyrimidinyl)hexahydro- (CA INDEX NAME)



IT 5767-37-3P, Hexamethylenimine, 1-(6-hydrazino-4-pyrimidinyl)-
RL: PREP (Preparation)
(preparation of)
RN 5767-37-3 HCAPLUS
CN 4(1H)-Pyrimidinone, 6-(hexahydro-1H-azepin-1-yl)-, hydrazone (9CI) (CA INDEX NAME)

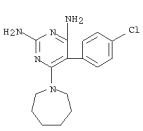


L21 ANSWER 24 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1959:40041 HCAPLUS
DN 53:40041
OREF 53:7214f-i
TI Pyrimidines
PA Societe des usines chimiques de Rhone-Poulenc
SO Addn. to Fr. 1,058,836 (C.A. 52, 16385a)
DT Patent
LA Unavailable
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI FR-----63159		19550825	FR	19520723 <--

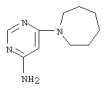
AB 2,4-Diaminopyrimidines containing 5-substituted phenyl and 6-substituted amino groups are prepared as in the main patent. Thus, 8 g. 2,4-diamino-5-(4-chlorophenyl)-6-chloropyrimidine autoclaved 7 hrs. at 200-10° with 16 cc. Bu2NH in 50 cc. EtOH give 2,4-diamino-5-(-4-chlorophenyl)-6-dibutylaminopyrimidine, m. 116-17° (aqueous EtOH); also obtained by autoclaving 2-amino-4-chloro-5-(4-chlorophenyl)-6-dibutylaminopyrimidine 6 hrs. at 200-10° with EtOH and NH3. Similarly are obtained derivs. bearing at position 6 the following groups: Me2N, m. 212-13°; Et2N, m. 208°; Pr2N, m. 129-30°; BuNH, m. 162-3°; piperidino, m. 190°; hexamethylenimino, m. 153°; 1-pyrolidinyl, m. 199-200°; Am2N, oil (hydrochloride m. 140-50°). Similarly Bu2NH and the 5-(3,4-dichlorophenyl) compound give 2,4-diamino-5-(3,4-dichlorophenyl)-6-dibutylaminopyrimidine, m. 106°. 2,4-Diamino-5-phenyl-6-chloropyrimidine (I) (37 g.) autoclaved 8 hrs. at 200° with 74 cc. EtOH and 200 g. NH3 gives, on cooling, adding 100 cc. EtOH, washing with H2O, taking up the insol. residue in 250 cc. N HCl, filtering, and basifying with NH4OH, 21 g. 2,4,6-triamino-5-phenylpyrimidine (II), m. 241° (EtOH); II treated with KNO3 in concentrated H2SO4 at -15° gives 2,4,6-triamino-5-(4-nitrophenyl)pyrimidine (III), m. 362-5° (hydrochloride m. 302-5°). III reduced over PtO2 gives 2,4,6-triamino-5-(4-aminophenyl)pyrimidine, m. 220°, solidifies and m. 238°; Sandmeyer reaction gives 2,4,6-triamino-5-(4-cyanophenyl)pyrimidine, m. 365-72°. I (48 g.) autoclaved 7 hrs. at 200° with 150 cc. EtOH and 113 g. Bu2NH gives, on cooling, taking up the solid in CHCl3, and adding excess dry HCl in Et2O, a dihydrochloride which, on recrystn. from H2O gives a monohydrochloride of 2,4-di-amino-5-phenyl-6-dibutylaminopyrimidine m. 194°, nitration of which gives 2,4-diamino-5-(4-nitrophenyl)-6-dibutylaminopyrimidine, m. 171°.

IT 131975-96-7P, Hexamethylenimine, 1-[2,6-diamino-5-(p-chlorophenyl)-4-pyrimidinyl]-
RL: PREP (Preparation)
(preparation of)
RN 131975-96-7 HCAPLUS
CN Hexamethylenimine, 1-[2,6-diamino-5-(p-chlorophenyl)-4-pyrimidinyl]- (6CI) (CA INDEX NAME)



L21 ANSWER 25 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1959:2101 HCAPLUS
DN 53:2101
OREF 53:390d-i,391a-f
TI Diuretics. Organomercurials. III. 4,6-Diaminopyrimidines
AU Whitehead, Calvert W.; Traverso, John J.
CS Lilly Research Labs., Indianapolis, IN
SO Journal of the American Chemical Society (1958), 80, 2185-9
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
AB Dry 4-amino-6-hydroxypyrimidine (111.1 g.) and 1200 cc. POCl3 treated with stirring with 160 g. PhNEt2, refluxed 4.5 hrs., the excess POCl3 distilled at 50-5° in vacuo, the residual thick brown sirup dissolved in an equal volume of Et2O, cooled in Dry Ice-Me2CO, treated dropwise with stirring with 200 cc. cold H2O at -10 to 0° with the pH maintained at approx. 6 with NH4OH, stirred 2 hrs., warmed to room temperature, adjusted to pH 6, and extracted 2-2.5 days with Et2O, the extract evaporated, the residue washed with petr. ether, dissolved in about 4 l. hot H2O, treated with C, cooled, and the precipitate filtered off (concentration of the mother liquors gave addnl. product) yielded 70-90 g. 4-amino-6-chloropyrimidine (I), m. 215°. I (5 g.) in 100 cc. absolute EtOH saturated with cooling with dry HCl yielded 4 g. I.HCl, m. 193° (decomposition) (EtOH). I (10 g.) and 0.14 mole appropriate alkylamine alone or in 50-100 cc. H2O, dioxane, EtOH, or PhMe refluxed 8-12 hrs. (low-boiling amines and I were heated at 110-20° in sealed tubes), cooled, filtered, concentrated, and the resulting precipitate recrystd. gave the corresponding 4-amino-6-(alkylamino)pyrimidines (II). I (10 g.) and 0.068 mole arylamine-HCl in 200 cc. dioxane and 30 cc. EtOH refluxed 24 hrs., cooled, the precipitate filtered off, dissolved in H2O, treated with C, the mixture filtered, basified with NH4OH, and the precipitated base recrystd. (aqueous EtOH) yielded the corresponding 4-amino-6-(substituted-amino)pyrimidines (III). By these procedures were prepared the following II and III (substituent on 6-amino group, % yield, m.p., and % diuretic activity given): Me, 62, 205°, 9; Et, 74, 193°, -; CH2:CHCH2, 65, 146°, 8; HO2C(CH2)2 (prepared by heating H2NCH2CH2CO2Na with I in H2O), 21, 225° (decomposition), -; Pr, 89, 140°, 15; iso-Pr, 81, 177°, 11; Bu, 78, 118°, 18 (pK'a 5.7); iso-Bu, 70, 125°, 16; furfuryl, 30, 172°, 11; Am, 72, 115°, 36; iso-Am, 50, 145°, 16; p-ClC6H4, 41, 179°, 40; Ph, 74, 179°, 100 (pK'a 4.9); 2-pyridylmethyl, 13, 188°, -; cyclohexyl, 54, 203°, 7; C6H13, 94, 115°, 11; m-MeC6H4, 35, 132°, 68; p-MeC6H4, 29, 175°, 100; PhCH2, 78, 211°, 69 (pK'a 5.0); p-MeOC6H4, 54, 215-20°, -; 1-hydroxycyclohexylmethyl, 70, 197°, - (pK'a 5.6); C7H15, 53, 119°, 16; o-ClC6H4CH2CH2, 47, 156°, -; Ph(CH2)2, 54, 164°, 13; MePhCH, 67, 171°, -; m-MeC6H4CH2, 94, 175°, 21; o-MeC6H4CH2, 90, 219°, -; p-MeC6H4CH2, 60, 206°, -; p-MeOC6H4CH2, 99, 131° (decomposition), -; PhO(CH2)2, 98, 190°, 86; 2-cyclohexylethyl, 60, 183°, -; C8H17, 76, 100°, -; 3,4-(CH2O2)C6H3(CH2)2, 55, 147°, -; Ph(CH2)3, 46, 107°, 38; p-MeOC6H4(CH2)2, 95, 165°, -; Ph(CH2)4, 98, 108°, -; 3,4-(MeO)2C6H3(CH2)2, 61, 152°, -; 3,4-(MeO)2C6H3(CH2)3, 45, 153°, -; PhC(C4H8)CH2, 48, 151°, -; Ph2CHCH2, 49, 143°, -. CH2[C(:NH)OEt]2 (23 g.) in 75 cc. absolute EtOH treated with 0.2 mole of the appropriate amine, the mixture shaken to solution, kept several days at room temperature, filtered, and the residue recrystd. (EtOH) yielded the corresponding CH2[C(:NH)NHR]22HCl (IV) (R, m.p. with decomposition, and % yield given): Et, 280°, 71; Bu, 290-5°, 49; CH2:CHCH2, 255°, 95; MeO(CH2)3, 230°, 59; C8H17, 280-90°, 78; furfuryl, 280°, 60; Ph(CH2)2, 300°, 61. The appropriate IV (0.05 mole) added with cooling to 5.4 g. NaOMe in 75 cc. EtOH, filtered, evaporated in vacuo, the residual sirup dissolved in 20 cc. HCO2Et, the solution kept 12 hrs. at room temperature, concentrated on the steam bath, cooled, and the crystalline deposit filtered off and recrystd. (50% EtOH) yielded the corresponding 4,6-bis(alkylamino)pyrimidines (alkyl group, % yield, m.p., and pK'a in 66% HCONMe2 given): Et, 79, 187°, 5.6; CH2:CHCH2, 19.5, 163°, 5.2; furfuryl, 14, 185°, 4.7; C8H17, 48, 112°, -. I (0.1 mole) treated in the usual manner with an appropriate secondary amine yielded the corresponding 4-amino-6-(substituted-amino)pyrimidines (6-substituent, % yield, and m.p. given): Me2N, 93, 202°;

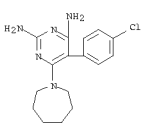
L21 ANSWER 25 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
1-pyrrolidinyl, 95, 243°; Et2N, 39, 132° (pK'a 5.7); morpholino, 72, 197°; piperidino, 97, 185°; homopiperidino, 81, 208° (pK'a 5.7); Pr2N, 33, 99°; MePhN, 82, 181°. 4,6-Dichloropyrimidine (V) (7.4 g.) mixed with 21.5 g. PhCH2NH2, heated 3 hrs. on the steam bath, dissolved in hot EtOH, and cooled gave 6.5 g. 4,6-bis(benzylamino)pyrimidine, m. 234-5°; the filtrate evapd., and the residue recrystd. (EtOAc-petr. ether) yielded 2 g. 4-benzylamino-6-chloropyrimidine, m. 121°. V (6.7 g.) and 14.6 g. BuNH2 gave similarly 6.7 g. 4,6-bis(butylamino)pyrimidine (VI), m. 154°. PhO(CH2)2NH2 (6.85 g.) in 60 cc. 20% EtOH heated 12 hrs. on the steam bath with 3.95 g. V and cooled yielded 6 g. 4-chloro-6-(2-phenoxyethylamino)pyrimidine, m. 98-100° (EtOAc-petr. ether). Furfurylamine (5.9 g.) and 4.46 g. V in 50 cc. H2O heated several hrs. on the steam bath and cooled yielded 3.5 g. 4-chloro-6-(furfurylamino)pyrimidine, m. 130° (EtOAc-petr. ether). Similarly was prepd. 4-chloro-6-piperidino-pyrimidine, m. 78°, 93%. VI (1 g.) and 1 g. MeI in 25 cc. EtOAc refluxed 1 hr. and cooled gave 1.2 g. VI.MeI, m. 121°, pK'a in 66% HCONMe2 12.8. The pK'a values were detd. in 66% HCONMe2 for the following compds.: 4-amino-6-(-phenyl-1-cyclopentylamino)pyrimidine 5.5, 4-amino-6-(N-methylanilino)pyrimidine 5.0. The diuretic activities were detd. by comparing the increase in urine vol./kg. body wt. over the normal output during 3 hrs., starting 1 hr. after dosage; the diuretic response was from doses of 5 and 10 mg./kg.; a value of 10% was obtained for a 20 mg./kg. dose of 1-allyl-3-ethyl-6-aminouracil. The LD50 values for the compds. tested varied between 500 and 1500 mg./kg. mice and rats.
IT 110378-52-4P, Hexamethylenimine, 1-(6-amino-4-pyrimidinyl)-
RL: PREP (Preparation)
(preparation of)
RN 110378-52-4 HCAPLUS
CN Hexamethylenimine, 1-(6-amino-4-pyrimidinyl)- (6CI) (CA INDEX NAME)



L21 ANSWER 26 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1956:4978 HCAPLUS
DN 50:4978
OREF 50:1094d-i
TI Substituted 5-phenylpyrimidines
PA Societe des usines chimiques de Rhone-Poulenc
DT Patent
LA Unavailable
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB----712595		19540728	GB	<--

GI For diagram(s), see printed CA Issue.
AB Pyrimidines of amebicidal activity have been prepared at 150-200° (or higher) in an organic solvent by action of NH3 or primary and secondary amines on a pyrimidine derivative C(NH2):N.C(NHR):N.CY:CC6H3XX'-4,3, where X and X' may be H, Cl, MeO, NH2, NO2, or CN, Y is a halogen atom, and R is H or an acyl radical. (In the product Y is replaced by the corresponding primary, secondary, or tertiary amino radical, especially straight chain C1-5 alkyl, piperidino, hexamethyleneimino, or pyrrolidino groups.) Thus, 8 g. 2,4-diamino-5-(4-chlorophenyl)-6-chloropyrimidine, 16 ml. Bu2NH, and 50 ml. EtOH were heated in a stirred autoclave 7 hrs. at 200-210°; the cooled mixture was filtered, washed with H2O and EtOH, and the residue was recrystd. from aqueous EtOH to yield 2,4-diamino-5-(4-chlorophenyl)-6-dibutylaminopyrimidine (I), m. 116-17°. In the same way, using other amines, the following 6-substituted pyrimidines were prepared: Mc2N m. 212-13°, Et2N m. 208°, Pr2N m. 129-30°, BuNH m. 162-3°, piperidino m. 190°, hexamethyleneimino m. 153°, pyrrolidino m. 199-200°, A2N m. 140-50°; also from 2,4-diamino-5-(3,4-dichlorophenyl)-6-chloropyrimidine, the corresponding 6-Bu3N derivative, m. 106°. Heating 5 g. 2-acetamido-4,6-dichloro-5-(4-chlorophenyl)pyrimidine (II), 80 ml. absolute EtOH, and 40 g. liquid NH3 6 hrs. at 200° gave 2.4 g. 2,4,6-triamino-5-(4-chlorophenyl)pyrimidine, m. 280-1° (from EtOH). Also from 37 g. 2,4-diamino-5-phenyl-6-chloropyrimidine (III), 74 ml. EtOH, and 200 g. NH3 was obtained 21 g. 2,4,6-triamino derivative m. 241°, which was converted by action of KNO3 on a solution of the compound in concentrated H2SO4 at -15° to 2,4,6-triamino-5-(4-nitrophenyl)pyrimidine (IV), m. 362-5°; HCl salt, m. 302-5°. IV was reduced with PtO2 to the 5-(4-aminophenyl) analog, m. 220°, resolidifies, m. again at 238°, which was converted to the corresponding nitrile, m. 365-72°, by the Sandmeyer reaction. Also, 48 g. III, 150 ml. EtOH, and 113 g. Bu2NH at 200° for 7 hrs. gave a residue which dissolved in CHCl3, from which a di-HCl salt was precipitated by HCl-Et2O addition which on recrystn. from H2O gave 2,4-diamino-5-phenyl-6-dibutylaminopyrimidine-HCl, m. 194°, which was nitrated to the 5-(4-nitrophenyl) compound, m. 171°. I was also prepared by heating 4 g. 2-amino-4-chloro-5-(4-chlorophenyl)-6-dibutylaminopyrimidine (V), 25 g. EtOH, and 24 g. NH3 6 hrs. at 200-10°; V, m. 147-8°, was made from II and excess Bu2NH at 110-15°.
IT 131975-96-7P, Hexamethylenlmine, 1-[2,6-diamino-5-(p-chlorophenyl)-4-pyrimidinyl]-
RL: PREP (Preparation)
(preparation of)
RN 131975-96-7 HCAPLUS
CN Hexamethylenimine, 1-[2,6-diamino-5-(p-chlorophenyl)-4-pyrimidinyl]- (6CI) (CA INDEX NAME)



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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate
substance identification.  Title keywords, authors, patent
assignees, and patent information, e.g., patent numbers, are
now searchable from 1907-1966.  TIFF images of CA abstracts
printed between 1907-1966 are available in the PAGE
display formats.

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FILE COVERS 1907 - 19 Feb 2008  VOL 148 ISS 8
FILE LAST UPDATED: 18 Feb 2008  (20080218/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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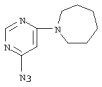
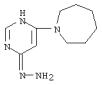
L27 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1966:93457 HCAPLUS
DN 64:93457
OREF 64:17589g-h,17590a
TI Tetrazole-azidoazomethine rearrangements in pyrimidine series
AU Postovskii, I. Ya.; Smirnova, N. B.
CS S. M. Kirov Polytech. Inst., Sverdlovsk
SO Doklady Akademii Nauk SSSR (1966), 166(5), 1136-9
CODEN: DANKAS; ISSN: 0002-3264
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB Addition of N2H4.H2O to 4,6-dichloropyrimidine in MeOH (exothermic) rapidly gave 66% 4-hydrazino-6-chloropyrimidine, m. 164-5°, which heated with aqueous amines 2 hrs. gave 65-70% 4-hydrazino-6-substituted-pyrimidines (substituent shown): morpholino, m. 166-7°; N-homopiperidinyl, m. 126-7°; N-pyrrolidinyl, m. 195-6°; piperidino, m. 122-3°. These treated with 2N HCl, followed by aqueous NaNO2 at 0°, gave 80-95% 4-azido-6-substituted-pyrimidines: morpholino, m. 92-3°; N-homopiperidinyl, m. 52°. The remaining enos were converted by this reaction into tetrazolo[c]-7-substituted-pyrimidines (I): N-pyrrolidinyl, m. 97°; piperidino, m. 77-8°. Ir spectra are shown. Thus, the presence of only electron-donor substituents leads to linear and cyclic nitrosation products. The tetrazole structures existed only in the solid state in the above products; in solution these were equilibrated with the azides (II), as shown spectroscopically
IT 5767-40-8
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 5767-40-8 HCAPLUS
CN 1H-Azepine, 1-(6-azido-4-pyrimidinyl)hexahydro- (CA INDEX NAME)



IT 5767-37-3P, Hexamethylenimine, 1-(6-hydrazino-4-pyrimidinyl)-
RL: PREP (Preparation)
(preparation of)
RN 5767-37-3 HCAPLUS
CN 4(1H)-Pyrimidinone, 6-(hexahydro-1H-azepin-1-yl)-, hydrazone (9CI) (CA INDEX NAME)



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L8            50 L5 SAM SUB=L7
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L11          933 L9 NOT L10

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L19            1 L18 AND C10H14N6
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L22            2 L10

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L23            0 L10
L24            3 L9
                 SEL HIT RN

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L25            4 E63-66
L26            1 L25 AND C10H17N5

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L27            1 L26 AND L24

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FILE COVERS 1907 - 20 Feb 2008 VOL 148 ISS 8
FILE LAST UPDATED: 19 Feb 2008 (20080219/ED)

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This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d bib abs hitstr l11 tot

L11 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:515487 HCAPLUS
DN 141:71555
TI Preparation of nitrogen-containing heterocyclic compounds as CXCR4 regulators
IN Habashita, Hiromu; Kokubo, Masaya; Shibayama, Shiro; Tada, Hideaki; Tanihiro, Tatsuya
PA Ono Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 641 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2004052862	A1	20040624	2003WO-JP15718	20031209
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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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EP----1571146	A1	20050907	2003EP-0778753	20031209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US2007167459	A1	20070719	2005US-0538758	20050610
PRAI 2002JP-0357446	A	20021210		
2003JP-0162706	A	20030606		
2003WO-JP15718	W	20031209		

OS MARPAT 141:71555
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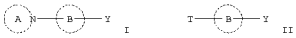
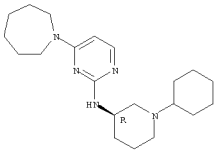


AB Compds. such as pyrimidine and quinazoline derivs. represented by the following general formulas (I) and (II), salts thereof, N-oxides thereof, solvates thereof or prodrugs of the same (wherein the ring A represents an optionally substituted nitrogen-containing heterocycle; the ring B represents an optionally substituted homocycle or an optionally substituted heterocycle; Y represents an optionally substituted hydrocarbyl group, an optionally substituted heterocyclic group, an optionally protected amino group, an optionally protected hydroxyl group or an optionally protected mercapto group; and T represents the ring A or an optionally substituted amino group) are prepared These compds. are CXCR4 regulators, in particular CXCR4 antagonists, and useful as preventives and/or remedies for various inflammatory diseases, immune diseases, various allergic diseases, infectious diseases, acquired immunodeficiency syndrome, infection with human immunodeficiency virus, psychiatric disorder, neurol. disease, cerebral diseases, cardiovascular diseases, metabolic diseases, or cancer, and agents for regeneration therapy, in particular transplant therapy. An assay system using SDF-1 which is an endogenous ligand of CXCR4 receptor, instead of HIV, was used in an assay for screening compds. which inhibit the binding of HIV to CXCR4 or CCR4 receptors on CD4-pos. cells. All the compds. prepared showed IC50 of 10 μM for inhibiting the binding of [125I]human SDF-1 to CEM cells, more specifically 0.1 μM for 2-(1-benzylpyrrolidin-3-ylamino)-4-(perhydroazepin-1-yl)pyrimidine. An ampule and tablet formulation containing 2-{[2-(dimethylamino)ethyl]amino}-4-(perhydroazepin-1-yl)pyrimidine were described.

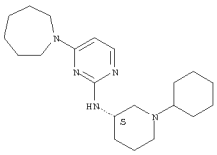
IT 710982-05-1P 710982-11-9P 710982-28-8P
710986-02-0P 711006-64-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

L11 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



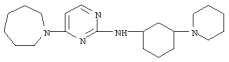
RN 711006-64-3 HCAPLUS
CN 2-Pyrimidinamine, N-[(3S)-1-cyclohexyl-3-piperidinyl]-4-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

Absolute stereochemistry.



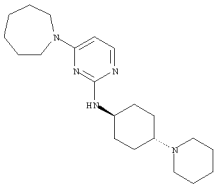
L11 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)

RN 710982-05-1 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-1H-azepin-1-yl)-N-[3-(1-piperidinyl)cyclohexyl]- (CA INDEX NAME)



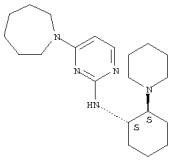
RN 710982-11-9 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-1H-azepin-1-yl)-N-[trans-4-(1-piperidinyl)cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 710982-28-8 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-1H-azepin-1-yl)-N-[(1R,2R)-2-(1-piperidinyl)cyclohexyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 710986-02-0 HCAPLUS
CN 2-Pyrimidinamine, N-[(3R)-1-cyclohexyl-3-piperidinyl]-4-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

Absolute stereochemistry.

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FILE LAST UPDATED: 19 Feb 2008  (20080219/ED)

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=> d bib abs hitstr l18 tot
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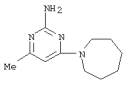
L18 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:1263574 HCAPLUS
DN 144:150323
TI Preparation of pyrimidine derivatives as potential medicinal agents by the reaction of 2-amino-4-chloro-6-methylpyrimidine with primary and secondary amines
AU Becker, Irwin
CS Department of Chemistry, Villanova University, Villanova, PA, 19085, USA
SO Journal of Heterocyclic Chemistry (2005), 42(7), 1289-1295
CODEN: JHTCAD; ISSN: 0022-152X
PB HeteroCorporation
DT Journal
LA English
OS CASREACT 144:150323
AB Thirteen derivs. of pyrimidine were prepared as potential medicinal agents by the reaction of 2-amino-4-chloro-6-(methyl)pyrimidine with primary and secondary amines in the absence of a solvent. Six of the derivs. are (piperazinyl)pyrimidine derivs. The compds. prepared in this work may prove to be efficacious in the treatment of inflammation, hypertension, anxiety, depression, or cancer (no biol. test data given).
IT 873839-06-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrimidine derivs. via reaction of (amino)chloro(methyl)pyrimidine with primary and secondary amines)
RN 873839-06-6 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-1H-azepin-1-yl)-6-methyl- (CA INDEX NAME)



RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:162059 HCAPLUS
DN 142:392365
TI Transformation of methyl N-methyl-N-(6-substituted-5-nitro-4-pyrimidinyl)aminoacetates into 4-methylamino-5-nitrosopyrimidines and 9-methylpurin-8-ones
AU Susvillo, Inga; Brukstus, Algirdas; Tumkevicius, Sigitas
CS Department of Organic Chemistry, Faculty of Chemistry, Vilnius University, Vilnius, LT-03225, Lithuania
SO Tetrahedron Letters (2005), 46(11), 1841-1844
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 142:392365
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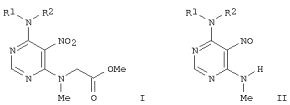
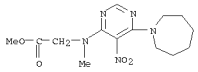


AB Upon treatment with sodium alkoxides, N-methyl-N-(6-amino-5-nitro-4-pyrimidinyl)aminoacetic acid Me esters I [R1 = H, Ph, 3-F3CC6H4, R2 = H; R1 = Me, R2 = MeO2CCH2, Ph; R1R2 = (CH2)6] undergo ring closure and rearrangement to give 6-substituted 4-methylamino-5-nitrosopyrimidines II or 9-methylpurin-8-ones III depending on the nature of substituents in the 6 position of the pyrimidine ring.
IT 850013-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amino(nitroso)pyrimidines and purinones by ring closure and rearrangement of (nitropyrimidinyl)aminoacetates under basic conditions)
RN 850013-78-4 HCAPLUS
CN Glycine, N-[6-(hexahydro-1H-azepin-1-yl)-5-nitro-4-pyrimidinyl]-N-methyl-, methyl ester (CA INDEX NAME)



RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:123192 HCAPLUS
DN 142:219313
TI Preparation of substituted pyrimidines as active ingredients of novel anthelmintic and insecticidal compositions
IN Lee, Byung Hyun; Larsen, Martha Jane; Kubiak, Teresa Maria
PA USA
SO U.S. Pat. Appl. Publ., 16 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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CA---2534975	A1	20050217	2004CA-2534975	20040726 <--
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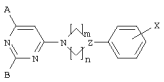
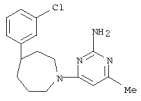
GI

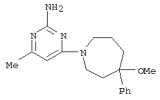


AB The title compds. I [A, B = H, alkyl, (un)substituted NH2, alkoxy; X = halo, alkyl, OH, etc.; m = 1-2; n = 1-3; when m and n are both 2, Z = N, CH, COR; when m and n are not both 2, Z = CH, COR; R = H, alkyl], useful for preventing or treating parasitic diseases, and for the prevention or treatment of parasites in a plant or agricultural crop, were prepared Thus, reacting 4-chloro-2,6-diaminopyrimidine with 4-phenylpiperidine in the presence of KI in DMF followed by treating the resulting free base with 0.5 M HCl in MeOH afforded 6-(4-phenylpiperidin-1-yl)pyrimidine-2,4-dione hydrochloride which showed inhibited motility of the H. contortus larvae at 10 μM. The composition comprising the one to three compds. I which is useful for preventing or treating parasitic diseases, is disclosed.
IT 841295-83-8P 841295-85-0P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrimidines as active ingredients of novel anthelmintic and insecticidal compns.)
RN 841295-83-8 HCAPLUS
CN 2-Pyrimidinamine, 4-[4-(3-chlorophenyl)hexahydro-1H-azepin-1-yl]-6-methyl- (CA INDEX NAME)

L18 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



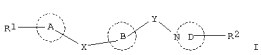
RN 841295-85-0 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-4-methoxy-4-phenyl-1H-azepin-1-yl)-6-methyl- (CA INDEX NAME)



L18 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:780666 HCAPLUS
DN 141:296046
TI Preparation of nitrogen-containing heterocyclic derivatives as chemokine receptor CCR5 antagonists and drugs containing the same as the active ingredient
IN Nishizawa, Rena; Takaoka, Yoshikazu; Shibayama, Shiro
PA Ono Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 306 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2004080966	A1	20040923	2004WO-JP03333	20040312 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NG, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU2004220225	A1	20040923	2004AU-0220225	20040312 <--
	CA---2517888	A1	20040923	2004CA-2517888	20040312 <--
	EP---1604981	A1	20051214	2004EP-0720257	20040312 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
	BR2004008332	A	20060321	2004BR-0008332	20040312 <--
	CN---1787996	A	20060614	CN 2004-80013002	20040312 <--
	NO2005004244	A	20051214	2005NO-0004244	20050913 <--
	ZA2005007365	A	20060628	2005ZA-0007365	20050913 <--
	IN2005DN04116	A	20071019	2005IN-DN04116	20050913 <--
	US2006178399	A1	20060810	2005US-0549120	20050914 <--
PRAI	2003JP-0070347	A	20030314	<--	
	2003JP-0385683	A	20031114	<--	
	2004WO-JP03333	A	20040312	<--	

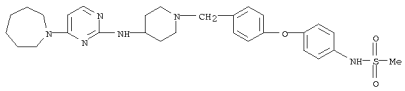
OS MARPAT 141:296046
GI



I

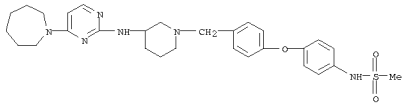
AB The title compds. [I; R1 = H, (un)protected acid group; X, Y = a bond, a spacer having 1-3 carbon atoms in the main chain; the ring A or B = (un)substituted 3- to 15-membered allocyclic or heterocyclic ring; the ring D = (un)substituted 3- to 15-membered N-containing heterocyclic ring; R2 = H, cyano, oxo, (un)protected HO, each (un)substituted hydrocarbyl, NH2, or 3- to 15-membered heterocyclyl, :N(OR6); wherein R6 = H, C1-4 alkyl] salts or solvates thereof or prodrugs thereof are prepared. These compds. are chemokine receptor CCR5 antagonists and useful in preventing and/or treating human immunodeficiency virus (HIV) infection (in particular, acquired immunodeficiency syndrome), immune diseases (in particular, rejection in organ transplantation), and various inflammatory diseases (in particular, asthma). The various inflammatory diseases may also include nephritis, nephropathy, hepatitis, arthritis, rheumatoid arthritis, rhinitis, conjunctivitis, and ulcerative colitis. The immunol. diseases may further include autoimmune diseases, psoriasis, and multiple sclerosis. They may be also useful for treating and/or preventing allergic diseases (atopic dermatitis, urticaria, allergic bronchopulmonary

L18 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
aspergillosis, or allergic eosinophilic gastroenteritis), ischemic reperfusion injury, acute respiratory distress syndrome, and shock accompanying bacterial infection, diabetes, cancer metastasis. Thus, a soln. of 500 mg 1-[4-[4-(methylsulfonylamino)phenoxy]benzyl]piperidine-4-carboxaldehyde, 396 mg N-(tert-butoxycarbonyl)-L-cyclohexylalanine, 0.140 mL n-butylamine, and 0.179 mL 2-morpholinoethyl isocyanide in 13 mL MeOH was stirred at 65° for 12 h, treated with 0.5 mL concd. HCl, stirred for 2 h, concd., treated with 15 mL CH2Cl2 and 15 mL satd. aq. NaHCO3, and extd. twice with CH2Cl2 to give, after workup, a residue which was heated with 1.25 M AcOH/EtOAc (20 mL) at 70° for 12 h to give, after workup and silica gel chromatog. and salt formation with HCl, N-[4-[4-[[4-[(5S)-1-butyl-5-(cyclohexylmethyl)-3,6-dioxopiperazin-2-yl]piperidin-1-yl]methyl]phenoxy]phenyl]methanesulfonamide hydrochloride. N-butyl-N-[1-[4-[4-(methylsulfonylamino)phenoxy]benzyl]piperidin-4-yl]cyclohexanecarboxamide hydrochloride (II) inhibited the human RANTES-induced temporary increase in cellular Ca2+ ion concn. in CHO stably expressing excess human CCR5 with IC50 of 0.077 μM. Pharmaceutical formulations, e.g. an ampule contg. II, were described.
IT 763932-38-3P 763932-39-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogen-containing heterocyclic derivs. as CCR5 antagonists for treating or preventing HIV infection, immune diseases, and inflammatory diseases)
RN 763932-38-3 HCAPLUS
CN Methanesulfonamide, N-[4-[4-[[4-[[4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]amino]-1-piperidinyl]methyl]phenoxy]phenyl]-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

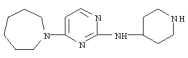
RN 763932-39-4 HCAPLUS
CN Methanesulfonamide, N-[4-[4-[[3-[[4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]amino]-1-piperidinyl]methyl]phenoxy]phenyl]-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

IT 763932-71-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen-containing heterocyclic derivs. as CCR5 antagonists for

L18 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
treating or preventing HIV infection, immune diseases, and inflammatory diseases)
RN 763932-71-4 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-1H-azepin-1-yl)-N-4-piperidinyl-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

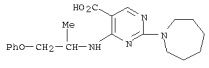
L18 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:531389 HCAPLUS
DN 141:99720
TI Preventives and/or remedies for central diseases
IN Mizoguchi, Ayumi; Sasaki, Katsutoshi; Hagihara, Koji; Aoyama, Shirou; Nonaka, Hiromi; Arai, Hitoshi; Shiozaki, Shizuo; Kuwana, Yoshihisa; Otsubo, Nobumasa
PA Kyowa Hakko Kogyo Co., Ltd., Japan
SO PCT Int. Appl., 169 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2004054617	A1	20040701	2003WO-JP15982	20031212 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU2003289330	A1	20040709	2003AU-0289330	20031212 <--
PRAI	2002JP-0362196	A	20021213	<--	
	2003WO-JP15982	W	20031212	<--	

OS MARPAT 141:99720
GI

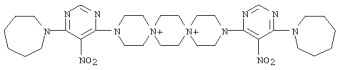
I

AB It is intended to provide a preventive and/or a remedy for central diseases containing, as the active ingredient, a substance having an effect of inhibiting the function of G-protein coupled receptor 88 (GPR88), and a pyrimidine derivative represented by the following general formula (I): I wherein A represents optionally substituted aryl, etc.; R1 represents hydrogen, etc.; R2 represents -NR3R4, etc.; X represents -C(=O)RS, etc.; and Y represents hydrogen, etc.; its pharmacol. acceptable salt, etc.
IT 714266-29-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(G-protein coupled receptor 88-inhibiting pyrimidine derivs., antibodies, and antisense oligonucleotides as preventives and/or remedies for central nervous system diseases)
RN 714266-29-2 HCAPLUS
CN 5-Pyrimidinecarboxylic acid, 2-(hexahydro-1H-azepin-1-yl)-4-[(1-methyl-2-phenoxyethyl)amino]- (CA INDEX NAME)



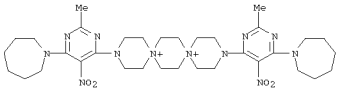
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2002:458417 HCAPLUS
DN 138:100338
TI Synthesis, cytotoxicity and antiviral activity of N,N'-bis-5-nitropyrimidyl derivatives of dispirotripiperazine
AU Schmidtke, M.; Riabova, O.; Dahse, H.-M.; Stelzner, A.; Makarov, V.
CS Institute of Virology, Friedrich Schiller University of Jena, Jena, D-07745, Germany
SO Antiviral Research (2002), 55(1), 117-127
CODEN: ARSRDR; ISSN: 0166-3542
PB Elsevier Science B.V.
DT Journal
LA English
AB During the search for new antivirals, various N,N'-bis-5-pyrimidyl derivs. of 3,12-diaza-6,9-diazonia(5,2,5,2)dispirohexadecane dichloride (dispirotripiperazine) were synthesized. To reveal relationships between chemical structure and antiviral activity, the compds. were characterized by fast atom bombardment mass, NMR, infra red spectroscopy, and elemental anal. and examined for cytotoxicity, inhibition of cell growth and antiviral activity under in vitro conditions. The results of this study demonstrate an excellent compatibility of the test compds. for confluent as well as proliferating cells and a potent structure-dependent inhibition of herpes simplex virus type 1 replication when added during viral adsorption. Functional group anal. revealed that both the dispirotripiperazine as well as the pyrimidine ring with a nitro group in the 5 position are necessary for activity. A reduction of electron d. in the terminal pyrimidine rings enhanced the antiviral activity whereas electron donor substitutions reduced it. Introduction of a Me group in position 2 of the pyrimidine had no influence on cytotoxicity or antiviral activity.
IT 488719-42-2 488719-43-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cytotoxicity and antiviral activity of bis(nitropyrimidyl) derivs. of dispirotripiperazine)
RN 488719-42-2 HCAPLUS
CN 3,6,9,12-Tetraazadispiro[5.2.5.2]hexadecan-6,9-ium, 3,12-bis[6-(hexahydro-1H-azepin-1-yl)-5-nitro-4-pyrimidinyl]-, chloride (1:2) (CA INDEX NAME)



●2 Cl-

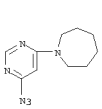
RN 488719-43-3 HCAPLUS
CN 3,6,9,12-Tetraazadispiro[5.2.5.2]hexadecan-9,6-ium, 3,12-bis[6-(hexahydro-1H-azepin-1-yl)-2-methyl-5-nitro-4-pyrimidinyl]-, chloride (1:2) (CA INDEX NAME)



●2 Cl-

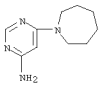
L18 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1966:93456 HCAPLUS
DN 64:93456
OREF 64:17589c-g
TI Resolution of several racemic barbitals into optical antipodes. III. Barbituric acid derivatives
AU Knabe, J.; Philipson, K.
CS Tech. Hochsch., Brunswick, Germany
SO Arch. Pharm. (1966), 299(3), 231-42
DT Journal
LA German
OS CASREACT 64:93456
GI For diagram(s), see printed CA Issue.
AB cf. CA 62, 16240g. The resolution of I (R = Et, R' = Ph, R'' = Me) (II) and I (R = iso-Pr, R' = CH2:CBrCH2, R'' = Me) (III) was achieved through the N-methylquininium salts. This method is also suitable for the resolution of N-unsubstituted barbitals with an asym. center in a C-5 side chain as demonstrated on the examples pentobarbital and vinylbital. II (246.3 g.) with N-methylquininium hydroxide (IV) in MeOH yielded 584.7 g. diastereomeric II-IV salts. II (9.81 g.) dissolved in 245.0 cc. MeOH containing 1 equivalent IV, concentrated to 1/3 volume and diluted with Et2O to turbidity gave 5.9 g. (+)-II-IV, m. 226° (MeOH-Et2O); the mother liquor diluted with Et2O gave 5.8 g. mixture and then 4.5 g. (-)-II-IV, m. 136° (MeOH-Et2O). (+)-II-IV (5.9 g.) in MeOH with 2N H2SO4 and H2O yielded 1.5 g. (+)-II, m. 101°, α20D 0.58° (c 3.118, absolute EtOH). (-)-II-IV (4.5 g.) gave similarly 1.0 g. (-)-II, m. 101°, α20D -0.50° (c 2.774, absolute EtOH). III (12.12 g.) in 245.0 cc. MeOH containing 1 equivalent IV yielded 8.9 g. (+)-III-IV, m. 238° (MeOH); the mother liquor yielded 6.1 g. mixture and 3.9 g. (-)-III-IV, m. 220° (MeOH-Et2O). (+)-III-IV (5.0 g.) in hot MeOH with 2N H2SO4 and H2O gave 1.1 g. (+)-III, m. 120°, α20D 0.54° (c 9.435, absolute EtOH). (-)-III-IV (3.9 g.) yielded similarly 1.0 g. (-)-III, m. 120°, α20D -0.50° (c 9.020, absolute EtOH). I (R = Et, R' = MePrCH, R'' = H) (V) with IV yielded 5.2 g. (-)-V-IV, m. 220° (MeOH-Et2O), 12.1 g. mixture, and 4.0 g. (+)-V-IV, m. 208° (MeOH-Et2O). (-)-V-IV (5.0 g.) in MeOH with H2SO4 yielded 1.5 g. (-)-V, m. 128°, α20D -0.13° (c 1.830, absolute EtOH). (+)-V-IV (4.0 g.) gave similarly 1.0 g. (+)-V, m. 128°, α20D 0.16° (c 2.608, absolute EtOH), 0.13° (c 2.086, CHCl3) ([α]20D 3.2°). I (R = CH2:CH, R' = MePrCH, R'' = H) (VI) (9.7 g.) with IV yielded 6.0 g. (-)-VI-IV, m. 218° (MeOH-Et2O), 11.3 g. mixture, and 6 g. oily (+)-VI-IV. (-)-VI-IV (6.0 g.) in MeOH wth H2SO4 yielded 1.1 g. (-)-VI, m. 94°, α20D -0.40 (c 4.275, absolute EtOH). (+)-VI-IV gave similarly 1.9 g. (+)-VI, m. 94°, α20D 0.32° (c 3.460, absolute EtOH). The ir spectra of (+)-II and (-)-II are recorded.
IT 5767-40-8
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 5767-40-8 HCAPLUS
CN 1H-Azepine, 1-(6-azido-4-pyrimidinyl)hexahydro- (CA INDEX NAME)

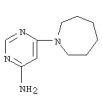


L18 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1959:2100 HCAPLUS
DN 53:2100
OREF 53:389c-i,390a-d
TI Diuretics. Organomercurials. II. Alkoxymercuration by mixed anion salts of mercury
AU Whitehead, Calvert W.; Traverso, John J.
CS Lilly Research Labs., Indianapolis, IN
SO Journal of the American Chemical Society (1958), 80, 2182-5
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
OS CASREACT 53:2100
GI For diagram(s), see printed CA Issue.
AB Hg(OAc)2 (3.18-15.9 g.) and an equimolar amount of HgCl2, HgBr2, HgI2, Hg(NO3)2, or Hg(SCN)2 were added to the appropriate alc. reactant or H2O; the resulting mixed mercuric salts were treated, without isolation, with the allylamides. The appropriate alkane-sulfonyl chloride added dropwise with stirring to 1 mole equivalent CH2:CHCH2NH2 or CH2:CHCH2NHMe in Et2O and 1 mole equivalent C5H5N, and the Et2O solution washed after 1 hr. with H2O, dried, and evaporated gave the corresponding amides; in the preparation of the H2O-soluble N-Me derivs., the Et2O solution was cooled and the C5H5N.HCl filtered off; in this manner were prepared the following RSO2NR'CH2CH:CH2 (I) (R, R', b.p./mm., and % yield given): Me, H, 103°/0.7, 72; Me, Me (II), 92°/0.5, 43; Et, H, 117-20°/0.5, 70; Bu, H (III), 114°/1.5, 68; Bu, Me (IV), 110°/0.5, 30. The appropriate N,N-dialkylsulfamoyl chloride (0.5 mole) added dropwise with stirring to 57 g. CH2:CHCH2NH2 in 500 cc. Et2O, and the mixture washed with H2O, dried, and distilled yielded the corresponding I (R' = H) (R, b.p./mm., and % yield given): Me2N, 110°/0.5, 9; EtMeN, 100°/0.5, 40; 1-pyrrolidinyl, 135°/0.7, 52; morpholino, - (m. 140°), 50; Et2N, 114°/1.5, 68. The appropriate I (0.1 mole) and 0.1 mole AcOHgCl in 200 cc. H2O or AcOHgBr in Me2CO warmed on the steam bath to about 60°, kept 4 days at room temperature, and filtered gave the corresponding RNHCH2CH(OR')CH2HgX (V) (R, R', X, m.p., and % yield given): MeSO2, H, Cl, 106°, 66; EtSO2, H, Br, 118°, 61; EtSO2, H, Cl, 84°, 90; 4-morpholinosulfonyl, Me, Cl (VI), 118°, 30. The products from II, III, and IV were oily and could not be characterized; the products from the I (R = dialkylamino) were sirups or plastics. CH2:CHCH2NH2 (250 cc.) and 132 g. H2NCONHCH2CO2Me refluxed 24 hrs., evaporated in vacuo, and the residue recrystd. (EtOH) yielded 140 g. H2NCONHCH2CONHCH2CH:CH2 (VII), m. 167-8°. VII (15.7 g.) stirred with 0.1 mole AcOHgCl in 200 cc. MeOH, AcOHgBr in 100 cc. MeOH, AcOHgSCN in 400 cc. MeOH, and AcOHgCl in 200 cc. H2O, kept 12 hrs. at room temperature, filtered, and each product recrystd. (MeOH) gave the following V (R = H2NCONHCH2CO) (R', X, m.p., and % yield given): H, Cl, 125-35° (decomposition), 42; Me, Br (IX), 174° (decomposition), 70; Me, Cl, 171° (decomposition), 90; Me, SCN (X), 132° (decomposition), 62. BzNHCH2CONHCH2CH:CH2 (5.5 g.) added to 0.025 mole AcOHgCl in 25 cc. H2O (and in 25 cc. MeOH), kept 3-5 days at room temperature, filtered, and the residue recrystd. (EtOH) gave the following V (R = BzNHCH2CO) (R', X, m.p., and % yield given): H, Cl (XI), 162°, 85; Me, Cl (XII), 99°, 98. 3-Allyl-5-carbethoxyuracil (XIII) (22.4 g.) and 155 cc. 1.3N NaOH treated dropwise with stirring at 40° with 12.6 g. Me2SO4, concentrated in vacuo, cooled, and the residue recrystd. (EtOAc-petr. ether) gave the 1-Me derivative (XIV) of XIII, m. 90°. HgCl (2.7 g.), 3.2 g. Hg(OAc)2, and 4.6 g. XIV in 50 cc. MeOH heated 5 min. on the steam bath, filtered, and cooled gave 7.5 g. 3-ClHgCH2CH(OMe)CH2 analog (XV) of XIV, m. 169° (MeOH). Hg(OAc)2 (3.2 g.), 2.76 g. Hg(SCN)2, 4.6 g. XIV, and 50 cc. MeOH warmed 5 min. at 50-60°, filtered, and cooled gave 5.1 g. 3-NCSHgCH2CH(OMe)CH2 analog (XVI) of XIV, m. 150-2°. 1,3-Dimethyl-5-carbethoxyuracil (100 g.), 300 cc. dioxane, and 60 cc. CH2:CHCH2NH2 heated overnight at 110° in a bomb, evaporated in vacuo, the residue dissolved in the min. amount of H2O, the aqueous solution treated with C, cooled, and the precipitate crystallized from a small volume of H2O yielded 40 g. 1,3-dimethyl-5-(N-allylcarbamoyl)uracil (XVII), needles, m. 133°. XVII (11.1 g.) heated to boiling with 0.05 mole each of AcOHgCl in 250 cc. H2O, AcOHgCl in 150 cc. MeOH, AcOHgCl in 150 cc. EtOH, AcOHgBr in 150 cc. MeOH, AcOHgI in 150 cc. MeOH, AcOHgNO3 in 150 cc. MeOH, AcOHgSCN in 150 cc. MeOH, AcOHgCl in 40 cc. MeO(CH2)2OH, cooled, kept at room temperature, filtered, and the residue recrystd. [(CH2Cl)2] yielded the following compds. (XVIII) (R, X, m.p., and % yield given): H, Cl (XIX), 166-8°, 88; Me, Br (XX), 204°, 90; Me, Cl (XXI), 215°, 62; Me, I (XXII), 184°, 95; Me, SCN (XXIII), 150-2°, 75; Et, Cl, (XXIV), (XVIII) 178-80°, 83; MeO(CH2)2O,

L18 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
Cl (XXV), 154°, 90. The apparent equil. consts. for the reaction RHgX + OH- .dblarw.RHgOH + X- at half-conversion were detd. in 66% HCONMe2 (the values in parentheses were detd. in H2O) for the following compds. (equil. const. given): IX, 2.1 + 103 (640); X, 7 + 105 (2.6-2.7 + 103); XI, 1.5 + 104 (1.4 + 104); XII, 0.9 + 104; XIX, 1.2 + 104 (1.0 + 104); XX, 1.1 + 103; XXI, 6.4 + 103; XXII, 47; XXIII, 2.3 + 105; XXIV, 8.1 + 103; XXV, 8.1 + 103; XV, 1.1 + 104 (0.9 104); XVI, 3.2 + 105; H2NCONHCH2CH(OMe)CH2HgI (XXVI), 130. XXVI, m. 165°, was prepd. in the standard manner in 70% yield.
IT 110378-52-4
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 110378-52-4 HCAPLUS
CN Hexamethylenimine, 1-(6-amino-4-pyrimidinyl)- (6CI) (CA INDEX NAME)



L18 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
31.8 g. VI and the ppt. washed with H2O, Et2O, and Et2O gave the corresponding p-(3-hydroxymercuri-2-alkoxypropoxy)benzoic acids (alkoxy group and % yield given): MeO, 68; HO(CH2)2O, 73; both acids decompd. on heating. p-H2NC6H4CH2CO2H (10.5 g.) and 8.3 g. MeCH:CHCOCl in aq. NaHCO3 yielded 9 g. p-MeCH:CHCONHC6H4CH2CO2H (IX), m. 206°. Similarly was prepd. p-MeCH:CHCONHC6H4CO2H, m. 268°, 70%. IX (1 g.), 1.5 g. VI, and 15 cc. (CH2OH)2 allowed to stand 5 days yielded 2 g. p-[2-(2-hydroxyethoxy)-3-(hydroxymercuri)butyrylamino]phenylacetic acid, m. 205° (decompn.). N-Allyl-N'-succinylurea (20 g.) in 40 cc. (CH2OH)2 treated with stirring with 32 g. VI, kept 2 days at room temp., distd. at 120°/0.1 mm., the sirupy residue dissolved in MeOH, treated with C, filtered, dild. with Et2O, the ppt. oil dissolved in the min. amt. of H2O, and the soln. adjusted with aq. NaOH to pH 7.5 and evapd. in vacuo yielded 60% N-[3-hydroxymercuri-2-(2-hydroxyethoxy)propyl]-N'-succinylurea Na salt. VI (6.4 g.) and 0.02 mole unsatd. compd. in 10-25 cc. of the appropriate alc. or 25 cc. H2O kept 2-5 days at room temp., filtered, and the residue recrystd. (EtOAc or EtOAc-petr. ether) gave the following p-Et2CC6H4OCH2CH(OR)CH2HgOAc (R, m.p., and % yield given): Me, 78°, 70; Et, 76°, 75; MeO(CH2)2, 52°, 78.
The following Et02CCH2OC6H4CONHCH2-CH(OR)CH2HgOX were prepd. (position of substituents on the benzene nucleus, R, X, m.p., and % yield given): o, Cl(CH2)2, H, 145°, 98; p, H, Ac (hydrate), 149°, 60; o, MeO(CH2)2, Ac, 107°, 67; p, Et02CMeCH, H, 110°, 55; o, EtO(CH2)2, Ac, 142°, 75; o, BuO(CH2)2, Ac, 145°, 70. Similarly were prepd. the following compds. (g. yield, and m.p. given): N-[3-acetoxymercuri-2-(2-methoxyethoxy)propyl]phthalimide(X), 9, 109°; 2-(2-hydroxymethoxy)propyl analog of X, 9.5, 126°; AcOHgCH2CH(OCH2CH2OH)CH2C(OH)Ph2, 4.5, 114.5°; AcOHgCH2CH(OMe)CH2C(OH)PH2 7.2, 135.6-36°; HO(CH2)2OCHPhCH(HgOH)CO2Me, 6.9, 216-18° (decompn.); MeO(CH2)2OCHPhCH(HgOAc)CO2Me, 7.9, 97°; Cl(CH2)OCHPbCH(HgOAc)2CO2Me, 7.5, 124°. 4,3-HO(CH2:CHCH2)C6H3CO2Et (2 g.) and 3.18 g. VI in 5 cc. (CH2OH)2 kept 3 days at room temp., dild. with Et2O, and filtered gave 4 g. 4,3-HO[AcOHgCH2CH(OCH2CH2OH)CH2]C6H3CO2Et, m. 99-100° (EtOAc-petr. ether). Similarly was prepd. in MeOH 4,3-HO[AcOHgCH2CH(OMe)CH2]C6H3CO2Et, m. 124-5°, 50%. In similar runs with EtOH, MeO(CH2)2OH, or PhCH2OH instead of (CH2OH)2 was formed 14-50% 2-acetoxymercuri-5-carbethoxy-2,3-dihydrobenzofuran, m. 114-16°.
IT 110378-52-4
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 110378-52-4 HCAPLUS
CN Hexamethylenimine, 1-(6-amino-4-pyrimidinyl)- (6CI) (CA INDEX NAME)



L18 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1959:2099 HCAPLUS
DN 53:2099
OREF 53:387h-i,388a-i,389a-c
TI Diuretics. Organomercurials
AU Whitehead, Calvert W.
CS Lilly Research Labs., Indianapolis, IN
SO Journal of the American Chemical Society (1958), 80, 2178-82
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
OS CASREACT 53:2099
AB The appropriate HOC6H4CO2Me (152 g.) and 124 g. CH2:CHCH2NH2 heated 12 hrs. in a sealed tube at 100-30°, cooled, diluted with cold H2O, acidified with HCl, extracted with Et2O, and the extract worked up gave the corresponding crude HOC6H4CONHCH2CH:CH2 (I) (position of OH group, m.p., and % yield given): m, 87°, 89; o, -, (oil), 71; p, -, 80.
The appropriate crude I (42 g.) and 26.5 g. ClCH2CO2H refluxed 2 hrs. with 34 g. NaOH in 2 l. H2O, treated again with 26.5 g. ClCH2CO2H and 17 g. NaOH, refluxed 1.5 hrs., cooled, and acidified with concentrated HCl, and the precipitate recrystd. (EtOH) gave the corresponding HO2CCH2OC6H4CONHCH2CH:CH2 (II) (position of HO2CCH2O group, % yield, and m.p. given): m, 99, 120°; p, 44, 139°; o, 70, 121.5°.
o-II (23.5 g.) and 100-300 cc. appropriate alcohol treated with stirring with 21.6 g. red HgO, heated 2-4 hrs. at 60°, filtered warm, the filtrate cooled, and the crystalline deposit recrystd. (EtOH or EtOH-HCONMe2) yielded the corresponding anhydro-o-(N-(3-hydroxymercuri)-2-(2-alkoxypropyl)carbamoyl)phenoxyacetic acid (alkoxy group, m.p., and % yield given): HO(CH2)2O (III), - (decomposition), 80; MeO(CH2)2O (IV), 135°, 52; BuO, 171°, 90; EtO(CH2)2O, 139°, 54; HO(CH2)2O(CH2)2O, 162°, 55; BuO(CH2)2O, 133°, 70; PhO(CH2)2O, 197°, 88; Et2CHCH2O(CH2)2O, 124°, 70; C10H21O, 164°, 39. In the preparation of IV the product was obtained as the MeO(CH2)2OH (V) solvate, m. 75°, which, recrystd. (EtOH) gave IV. m-II (4.8 g.), 6.4 g. Hg(OAc)2 (VI), and 25 cc. V allowed to stand 3 days, diluted with petr. ether, filtered, and the residue washed with EtOH and then Et2O yielded 7 g. m-isomer of IV; it did not have an identifying m.p. m-II (4.8 g.), 6.4 g. VI, and 25 cc. (CH2OH)2 allowed to stand 3 days diluted with H2O, and the gummy precipitate triturated with EtOH and with Et2O yielded 7.5 g. amorphous m-isomer of III. p-II (4.8 g.), 6.4 g. VI, and 40 cc. (CH2OH)2 gave 7 g. p-(N-[3-acetoxymercuri-2-(2-hydroxyethoxy)propyl]carbamoyl)phenoxyacetic acid, m. 145° (EtOH).
Dry BuOH (75 cc.), 5.2 g. 2-nonenoic acid, and 10.6 g. VI stirred until dissolved, allowed to stand a few hrs., filtered, and the residue washed with hot MeOH yielded 10 g. anhydro-3-butoxy-2-(hydroxymercuri)nonanoic acid, m. 186-8° (decomposition). Ph(CH2)2CH:CHCO2H (8.8 g.) in 50 cc. MeOH and 15.9 g. VI stirred to solution, kept 0.5 hr. at room temperature, filtered, and the residue washed with MeOH yielded 15 g. anhydro-2-hydroxymercuri-3-methoxy-5-phenylpentanoic acid, m. 189-90°. p-HOC6H4CH2CO2Et (97 g.) and 45 g. CH2:CHCH2NH2 refluxed 24 hrs., evaporated in vacuo, the residual sirup dissolved in the min. amount of warm EtOAc, and the solution diluted with petr. ether to incipient turbidity yielded 86 g. p-HOC6H4CH2CONHCH2CH:CH2 (VII), m. 84° [(CH2Cl)2].
VII (0.1 mole) treated with 18.8 g. ClCH2CO2H in aqueous NaOH yielded 29 g. p-HO2CCH2OC6H4CH2CONHCH2CH:CH2 (VIII), m. 137-9°. VII (50 g.), 32 g. ClCH2CO2Et, and 71 g. K2CO3 in 500 cc. Me2CO refluxed 48 hrs., evaporated, and the residual sirup crystallized from EtOAc and petr. ether yielded 51 g. Et ester of VIII, m. 86°. m-I (48 g.), 44 g. ClCH2CO2Et, and 50 g. K2CO3 in 300 cc. Me2CO yielded 40 g. Et ester of m-II, b1 204°.
p-II (89 g.) in 1 l. absolute EtOH refluxed 12 hrs. with 30 cc. concentrated H2SO4, evaporated in vacuo, and the residue poured onto 1 kg. ice and filtered yielded 83 g. Et ester of p-II, m. 104-5° (EtOAc-petr. ether). The Et ester of o-II, m. 78°, was prepared similarly in 80% yield. p-HSC6H4SO3H (128 g.) and 64.6 g. ClCH2CO2H heated several hrs. on the steam bath with 81 g. NaOH in 500 cc. H2O, cooled, and filtered gave 266 g. di-Na salt of p-HO3SC6H4SCH2CO2H; the salt kept 24 hrs. with POCl3 at room temperature, refluxed 2 hrs., evaporated in vacuo, and the residual oil stirred 1 hr. with cold H2O yielded 106 g. p-ClO2SC6H4CH2CO2H; a 26.6-g. portion with 5.7 g. CH2:CHCH2NH2 gave 16 g. p-CH2:CHCH2NHO2SC6H4SCH2CO2H, m. 129-30°. p-CH2:CHCH2OC6H4CO2H (17.8 g.) in 75 cc. of the appropriate alc. allowed to stand at room temperature with

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     (FILE 'HOME' ENTERED AT 13:08:43 ON 20 FEB 2008)

     FILE 'HCAPLUS' ENTERED AT 13:08:54 ON 20 FEB 2008
L1            1 US20070167459/PN

     FILE 'REGISTRY' ENTERED AT 13:09:18 ON 20 FEB 2008

     FILE 'HCAPLUS' ENTERED AT 13:09:18 ON 20 FEB 2008
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     FILE 'REGISTRY' ENTERED AT 13:09:19 ON 20 FEB 2008
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                  ACT J758C4A/A
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L4                STR
L5   (       3911)SEA FILE=REGISTRY ABB=ON  PLU=ON  NC6/ES AND NCNC3/ES
L6           2301 SEA FILE=REGISTRY SUB=L5 SSS FUL L4
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L7           1368 L6 AND L3
L8             20 L6 AND C21H35N5
L9             12 L8 AND NC6/ES AND C6/ES AND NCNC3/ES
L10             5 L9 AND NC5/ES

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     FILE 'REGISTRY' ENTERED AT 13:15:50 ON 20 FEB 2008
L12           933 L6 NOT L7

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L15             30 L14 AND PD<=20040610
L16             26 L15 AND L13 (L) PREP+NT/RL
L17             14 L14-15 NOT L16
                   SEL AN 4 7-14
L18              9 E214-231 AND L17

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